Sparse supernodal solver using block low-rank compression: Design, performance and analysis

November 21th, 2019 - JOREK development meeting - Cadarache

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Context - PhD of Gregoire Pichon and Esragul Korkmaz

Current sparse direct solvers for 3D problems of size n

- $\Theta(n^2)$ time complexity
- $\Theta(n^{\frac{4}{3}})$ memory complexity
- BLAS Level 3 operations with computations on blocks

Low-rank compression in sparse direct solvers

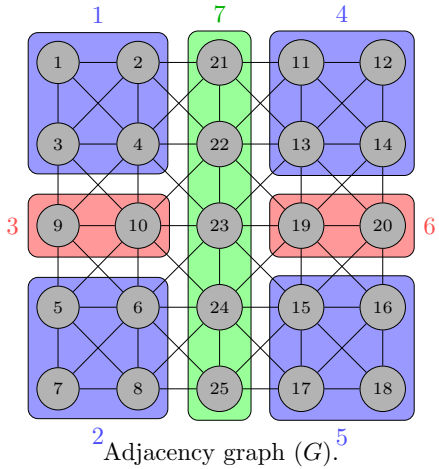
- Compress diagonal and off-diagonal blocks
- Use different compression formats: BLR, $\mathcal{H}$, HODLR, HSS, $\mathcal{H}^2$..
- Recently introduced in many solvers: MUMPS, PASTIX, STRUMPACK and many others

Objective of this talk: study low-rank clustering strategies to enhance blocks compressibility in the Block Low-Rank (BLR) case

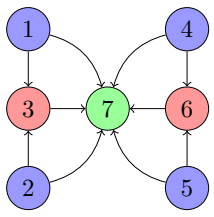
Symbolic Factorization

General approach

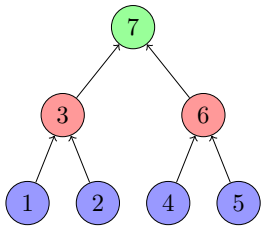
1. Build a partition with the nested dissection process
2. Compress information on data blocks
3. Compute the block elimination tree using the block quotient graph



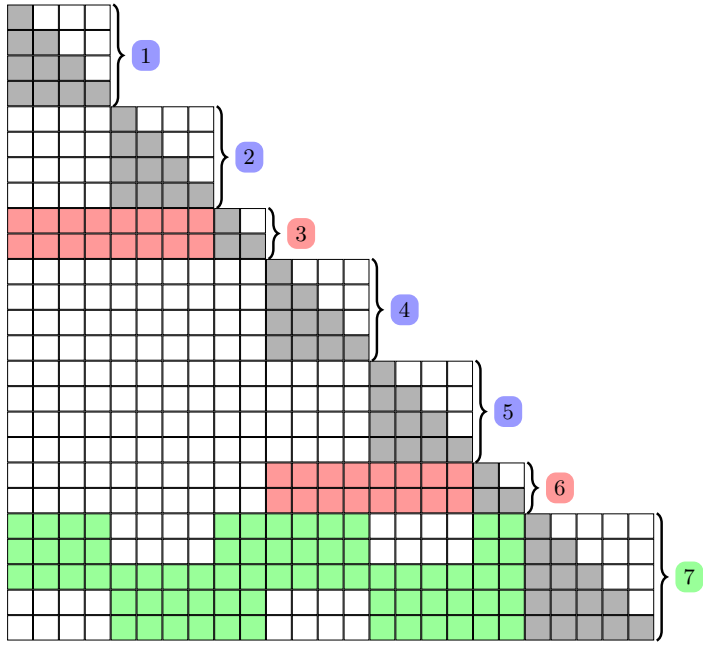
Adjacency graph (G).



Quotient graph (G^*/P) $= (G/P)^*$

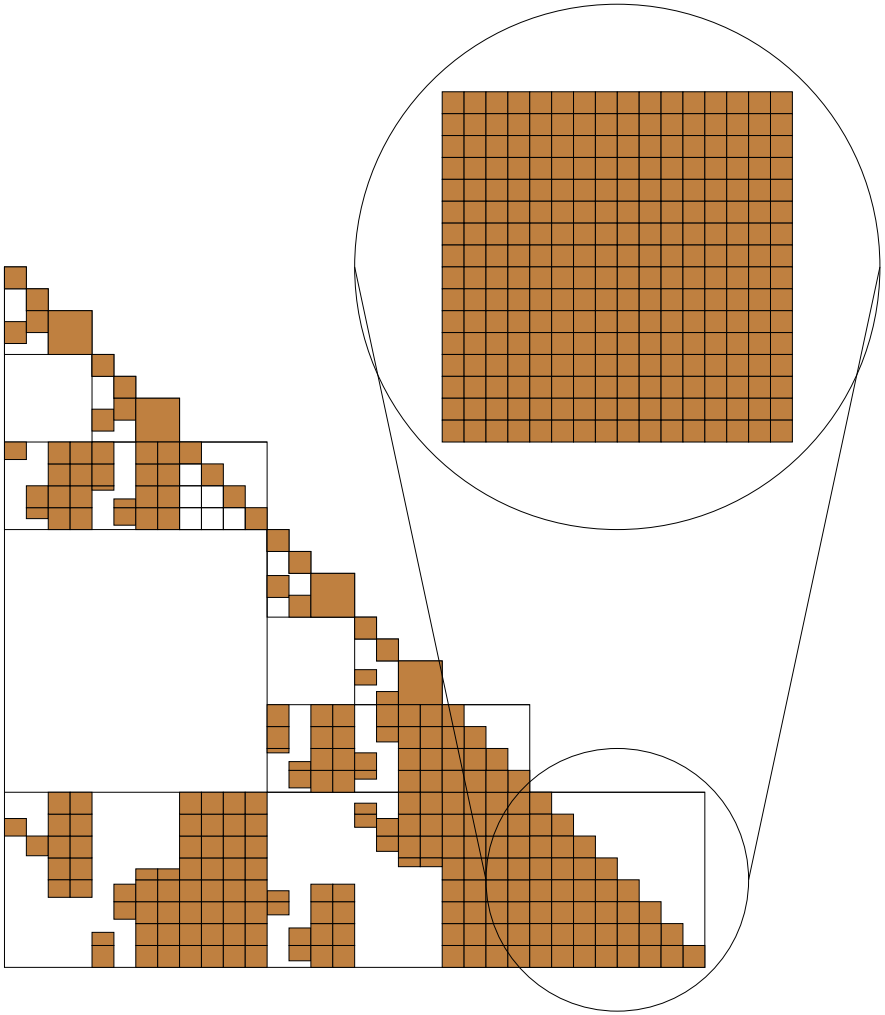


Elimination tree (T).



Factorized matrix (L).

BLR compression – Symbolic factorization



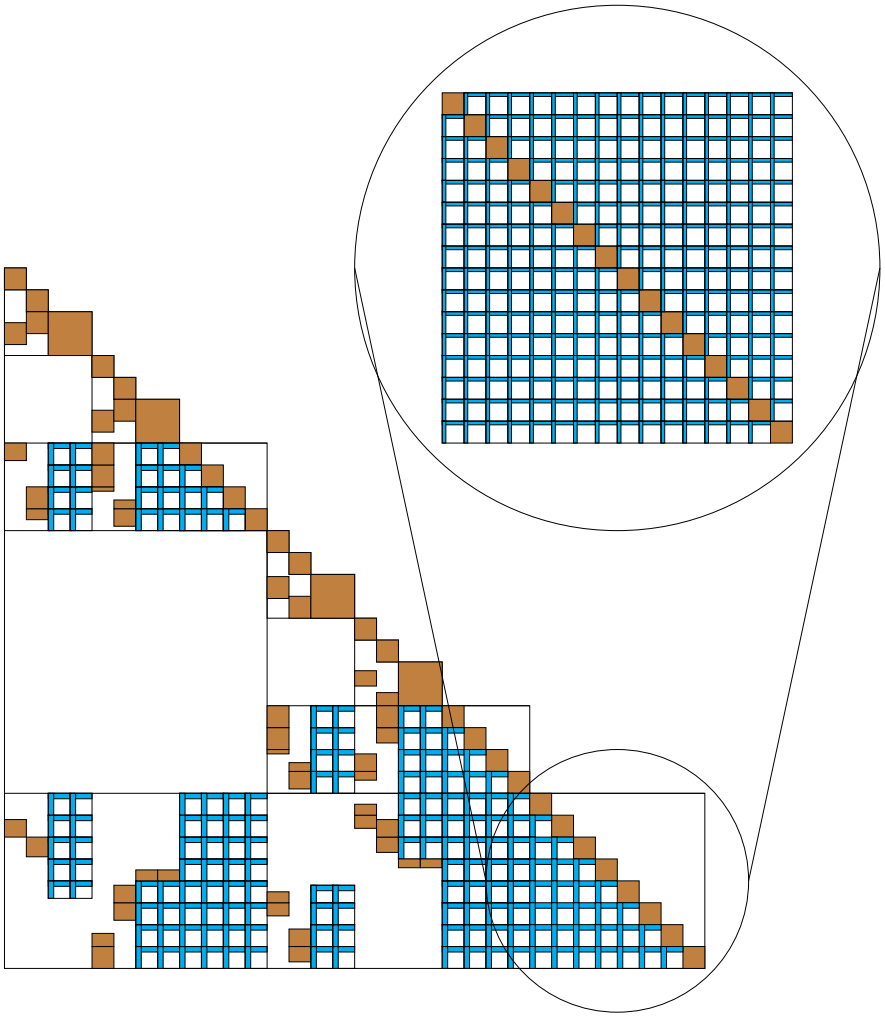
Approach

- Large supernodes are split
- It increases the level of parallelism

Operations

- Dense diagonal blocks
- TRSM are performed on dense off-diagonal blocks
- GEMM are performed between dense off-diagonal blocks

BLR compression – Symbolic factorization



Approach

- Large supernodes are split
- Large off-diagonal blocks are **low-rank**

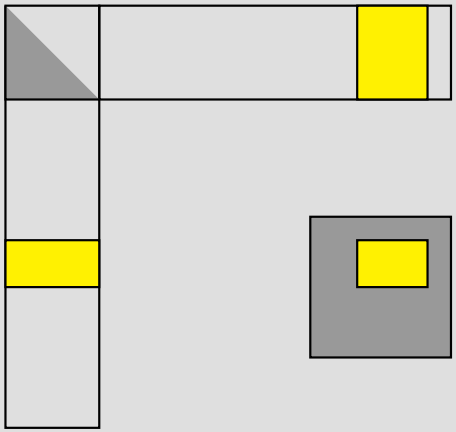
Operations

- Dense diagonal blocks
- TRSM are performed on **low-rank** off-diagonal blocks
- GEMM are performed between **low-rank** off-diagonal blocks

Summary of the possible updates

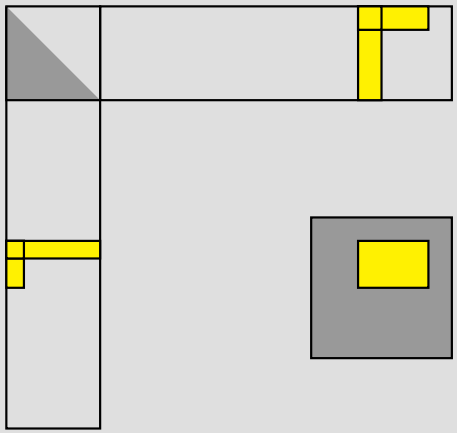
Cost of applying a $m \times n$ update to a $M \times N$ block.

Full rank



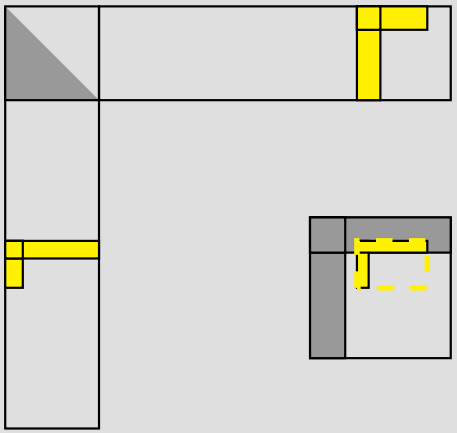
- A single GEMM kernel
- Cost depends on mn

Just-In-Time (non-fully structured)



- Serie of small GEMM kernels
- Cost depends on mn

Minimal Memory (fully structured)



- Complex extend-add operation
- Cost depends on MN

Can we reduce the number small updates, especially for fully structured case?

Compression kernels

Kernel	Complexity
Singular Value Decomposition (SVD)	$\Theta(mn^2)$
Rank-Revealing QR (RRQR)	$\Theta(mnr)$
RRQR with randomization	$\Theta(mnr)$
ACA, BDLR, CUR	$\Theta((m+n)r)$

Properties

- SVD provides the best ranks at a given accuracy with $||.||_2$
- RRQR keeps a control of accuracy, but efficiency is poor due to pivoting
- Randomization techniques are suitable to perform a rank-r approximation but may be costly for computing an accurate representation
- The accuracy of ACA/BDLR/CUR is problem dependent

Experimental setup

Machine: 2 INTEL Xeon $E5-2680v3$ at 2.50 GHz

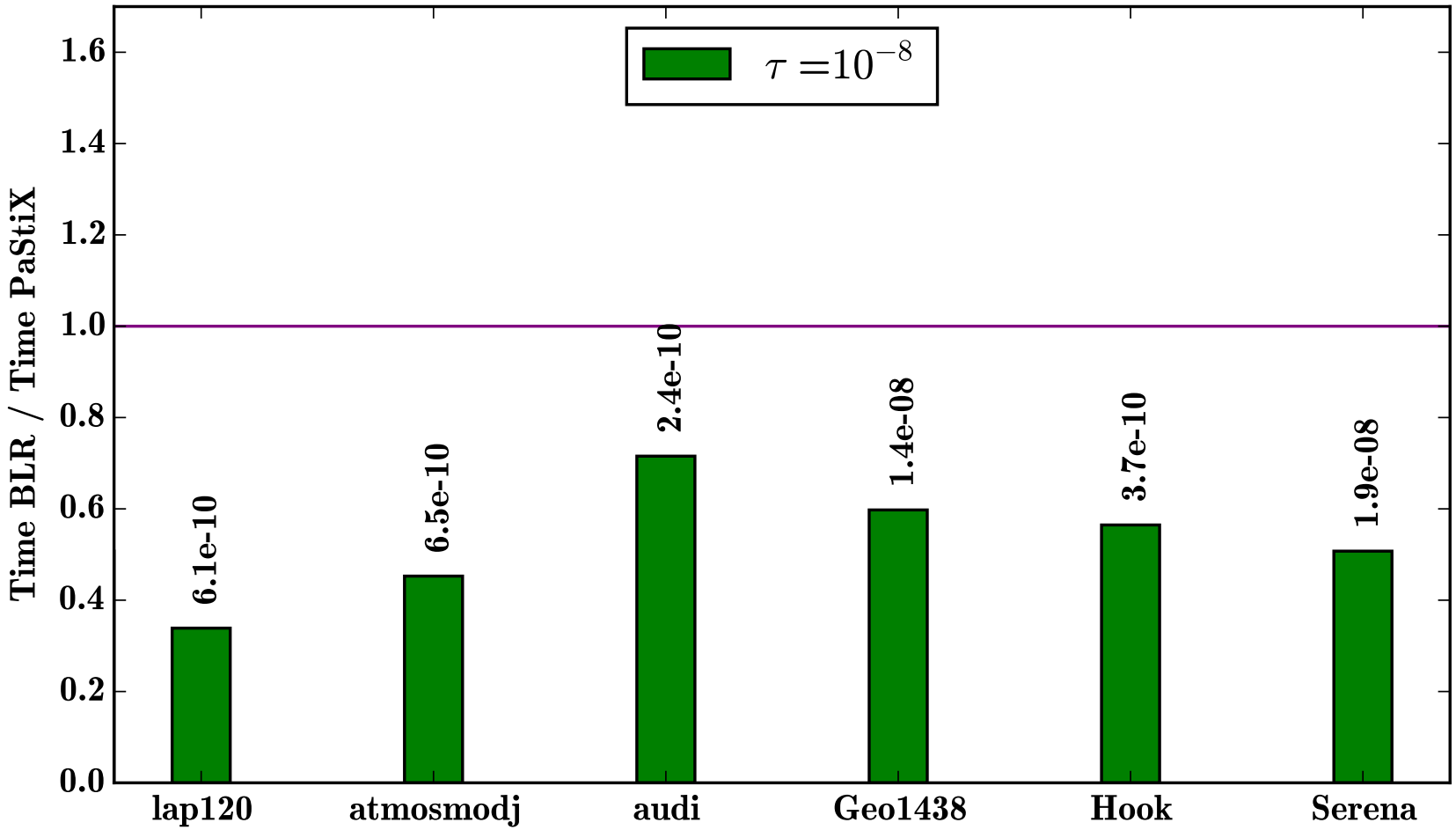
- 128 GB
- 24 threads
- Parallelism is obtained following PASTIX static scheduling for multi-threaded architectures (PARSEC version will be discussed later)

Entry parameters

- Tolerance τ: absolute parameter (normalized for each block)
- Compression method is RRQR
- Blocking sizes: between 128 and 256 in following experiments

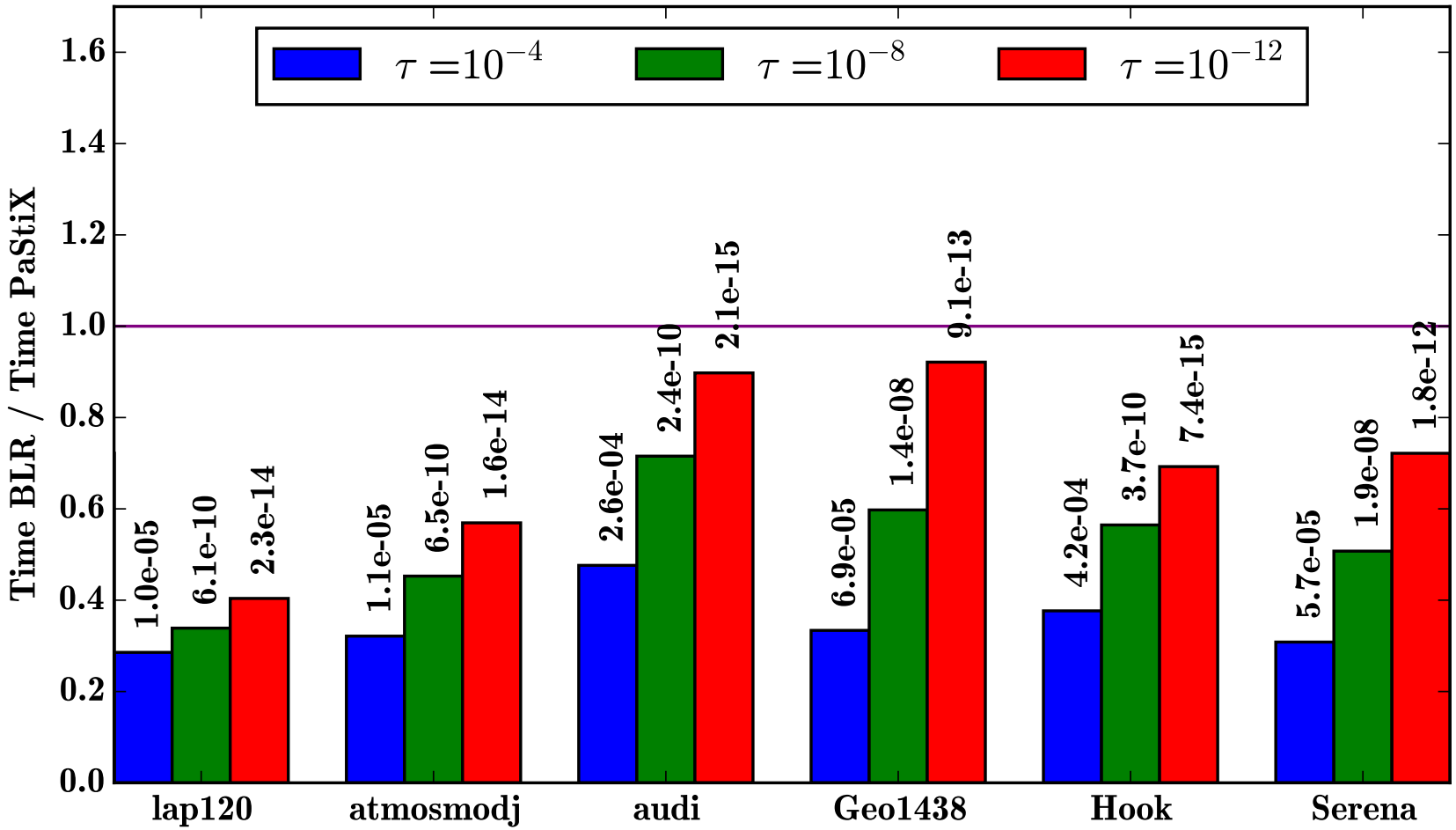
Matrix	Fact.	Size	Field
lap120	LDL^t	120^3	Poisson problem
Atmosmodj	LU	1 270 432	atmospheric model
Audi	LL^t	943 695	structural problem
Geo1438	LL^t	1 437 960	geomechanical model of earth
Hook	LDL^t	1 498 023	model of a steel hook
Serena	LDL^t	1 391 349	gas reservoir simulation

Performance of RRQR/Just-In-Time wrt full-rank version



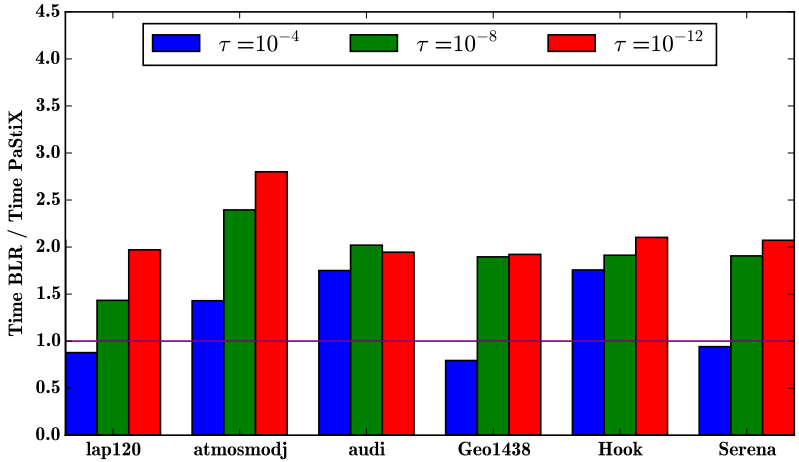
Factorization time reduced by a factor of 2 for $\tau = 10^{-8}$

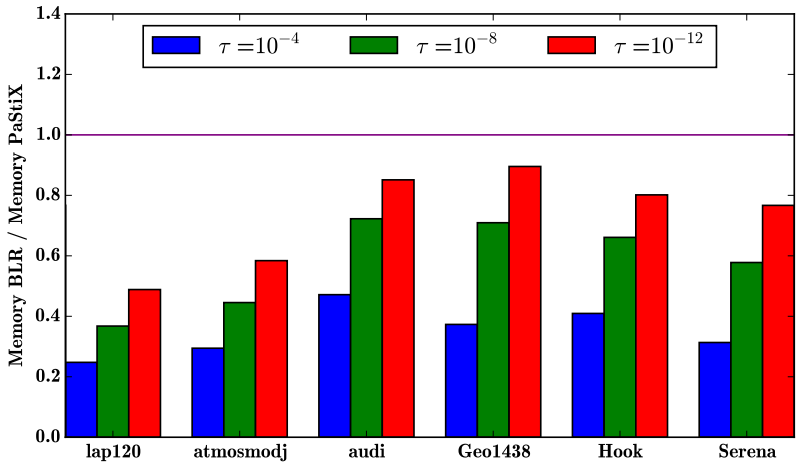
Performance of RRQR/Just-In-Time wrt full-rank version



Factorization time reduced by a factor of 2 for $\tau = 10^{-8}$

Behavior of RRQR/Minimal Memory wrt full-rank version





Performance

- Increase by a factor of 1.9 for $\tau = 10^{-8}$
- Better for a lower accuracy

Memory peak

- Reduction by a factor of 1.7 for $\tau = 10^{-8}$
- Close to the results obtained using SVD

Related work

BLR

MUMPS BLR compression in a multifrontal solver with dense assembly, which can perform pivoting

Hierarchical

H-LIB Hierarchical matrices for sparse by Hackbusch et al. which does not exploit all structural zeroes

Hmat-OSS A. Falco's thesis that uses hierarchical matrices together with a symbolic factorization

CHOLMOD Supernodal solver using randomization with fixed rank

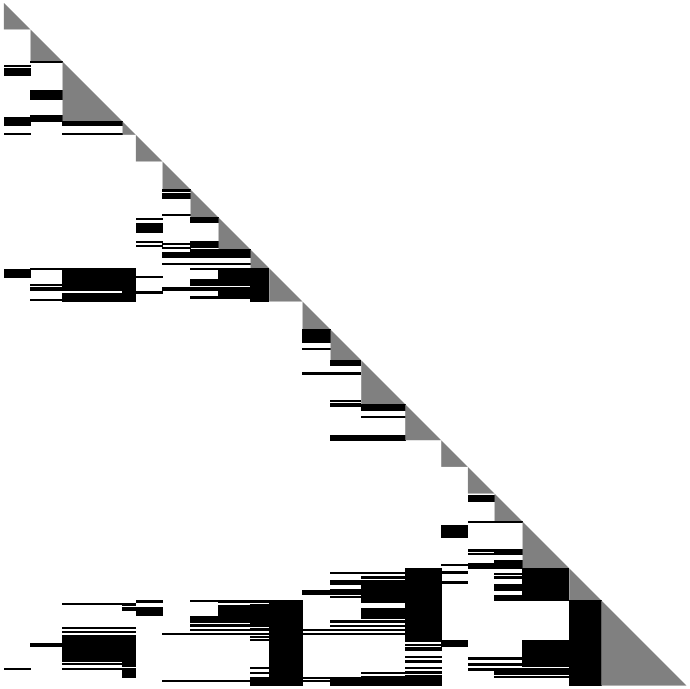
STRUMPACK HSS by Ghysels et al. with randomized sampling

Many other solvers

- Weak admissibility: HODLR, HSS
- Nested bases: HSS, $\mathcal{H}^2$
- Often used as preconditioners

Ordering for sparse matrices

One can reorder separators without modifying the fill-in



Symbolic factorization of a $8 \times 8 \times 8$ Laplacian

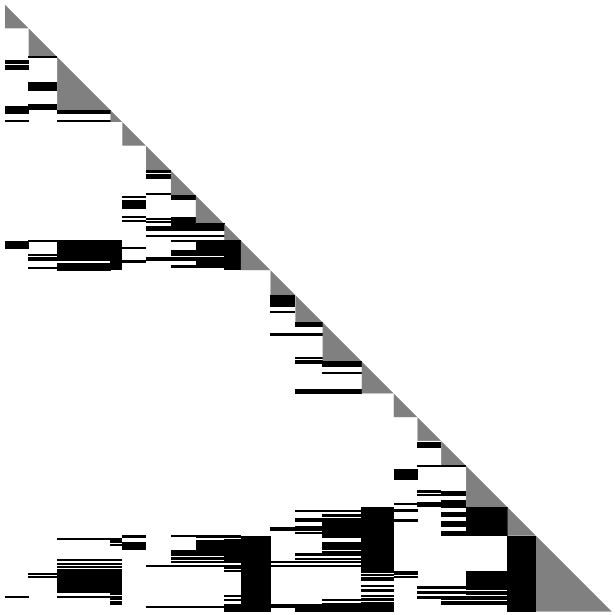
Enhance ordering

- Modify the partitioning process to enhance compressibility
- Reorder unknowns within a separator:
  - To enhance clustering within the separator
  - To enhance the coupling part

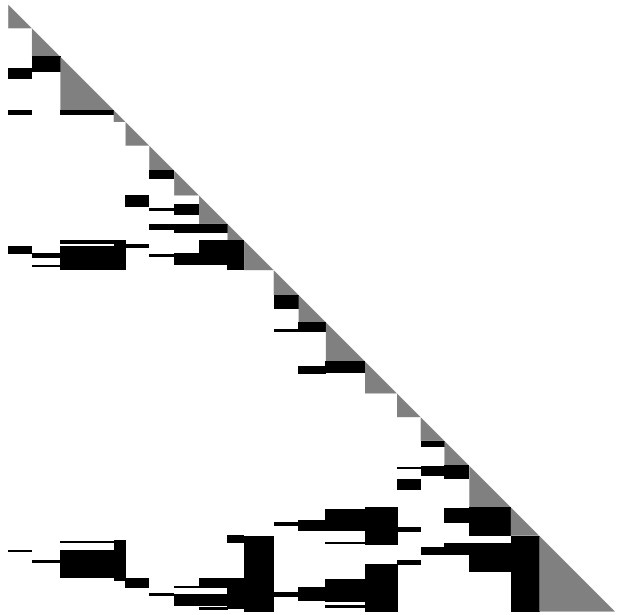
Reordering to minimize the number of off-diagonal blocks

Proposition

- Ordering of separators to minimize the number of off-diagonal blocks
- Does not impact memory consumption or the number of operations
- Increase granularity
  - Reduce the number of low-rank updates
  - Enhance the use of heterogeneous architectures (GPUs, Xeon Phi)



Without reordering (RCM)



With reordering

Reordering results

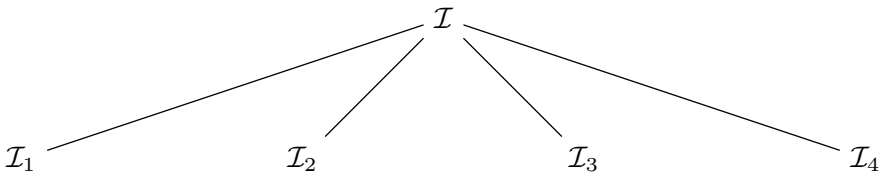
Summary

- Reduce the number of off-diagonal blocks and thus the overhead associated with low-rank updates
- Lead to larger data blocks suitable for modern architectures
- Always increase performance wrt SCOTCH

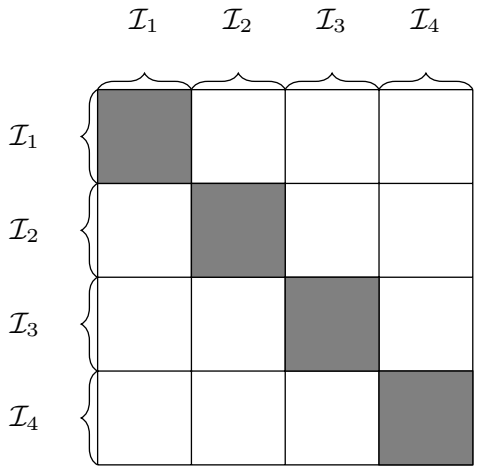
Architecture	Nb. units	Mean gain	Max gain
Westmere	12 cores	2%	6%
Xeon E5	24 cores	7%	13%
Fermi	12 cores + 1 to 3 M2070	10%	20%
Kepler	24 cores + 1 to 4 K40	15%	40%
Xeon Phi	64 cores	20%	40%

Performance gain for the full-rank factorization when using PARSEC runtime system with TSP instead of SCOTCH

BLR clustering for a dense matrix



Cluster tree



Flat clustering

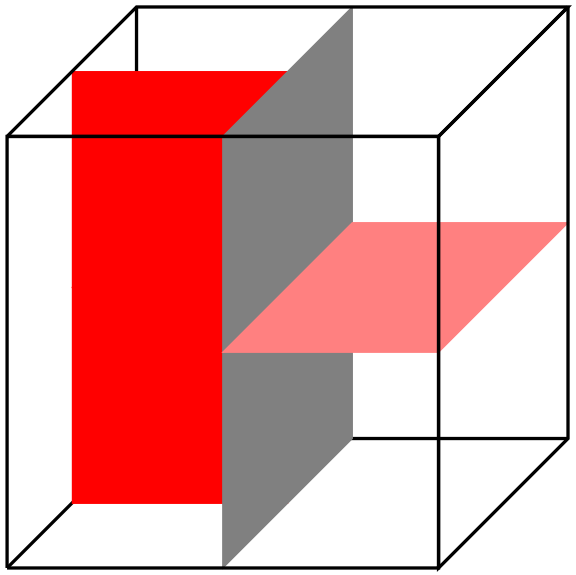
$\sigma \times \tau$ is admissible $\iff \max(\text{diam}(\sigma), \text{diam}(\tau)) \leq \eta \, \text{dist}(\sigma, \tau)$

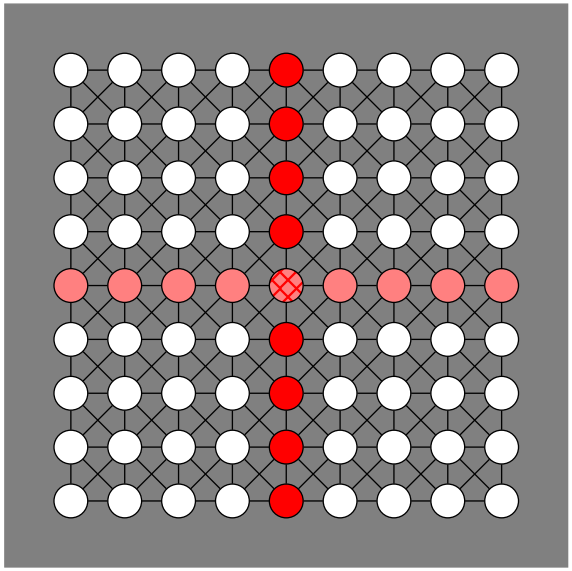
Can be computed with the knowledge of geometry; otherwise, k-way partitioning can be used for clustering separators

Towards sparse ordering dedicated to low-rank

Nested dissection

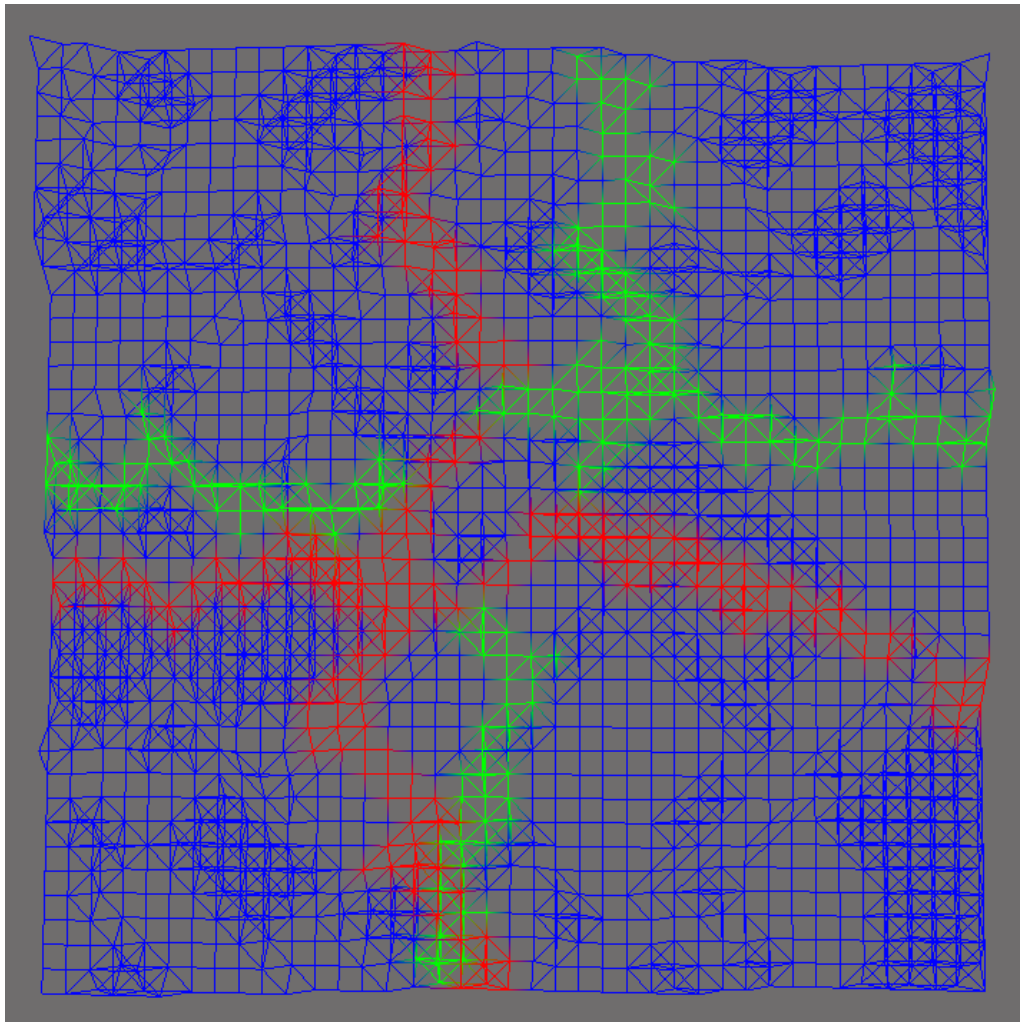
1. Partition $V = A \cup B \cup C$
2. Order C with larger indices: $V_A < V_C$ and $V_B < V_C$
3. Apply the process recursively on A and B





As A and B are processed independently, their interaction with C is not the same, even for a perfect nested dissection of a $N \times N \times N$ cube

Example on a cube partitioned with SCOTCH



First separator of a $40 \times 40 \times 40$ Laplacian partitioned with SCOTCH

Suitable clustering strategy

Let us consider the last separator A_{22} and its interactions with previous supernodes A_{11}:

$$\begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}$$

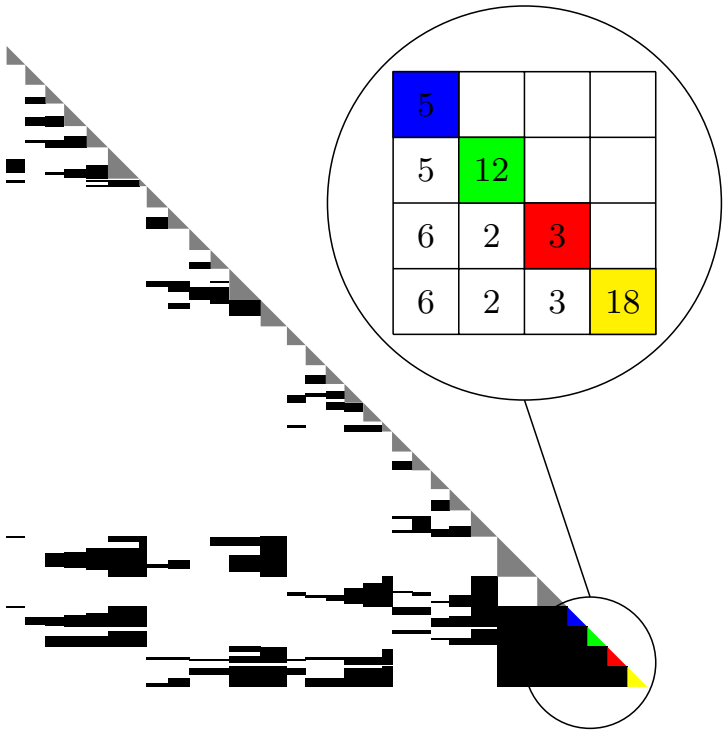
Existing approaches

- K-way partitioning orders correctly A_{22}
- The reordering strategy reduces the number of off-diagonal blocks in A_{12} and A_{21}

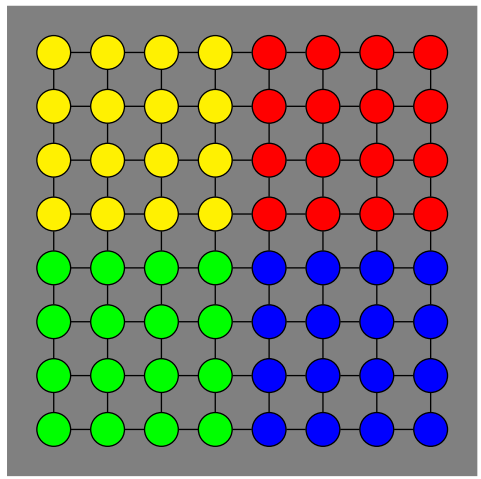
We introduce a new strategy to couple the advantages of both approaches, with suitable structure for both intra and inter separators blocks

Clustering techniques: existing solutions

- k-way partitioning (dense, multifrontal)



(a) Symbolic factorization

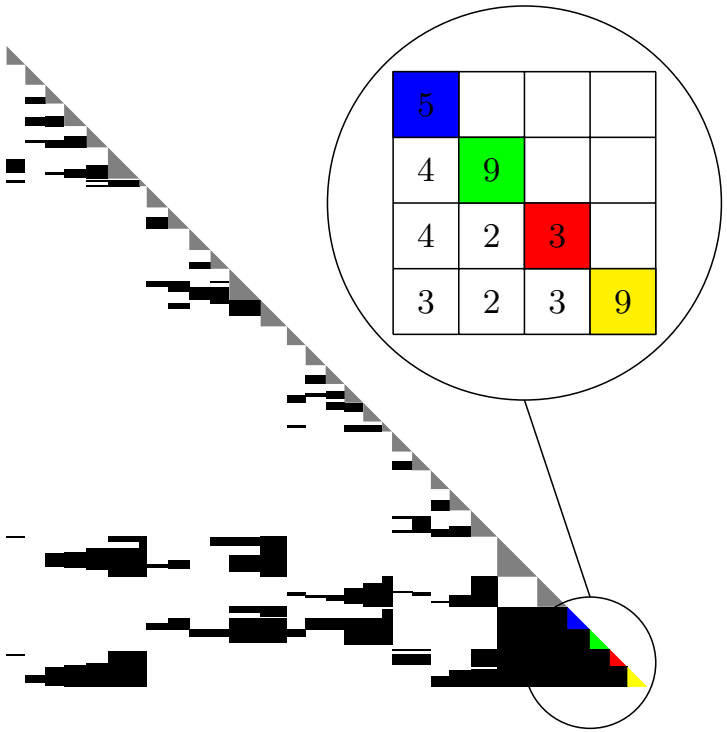


(b) First separator clustering

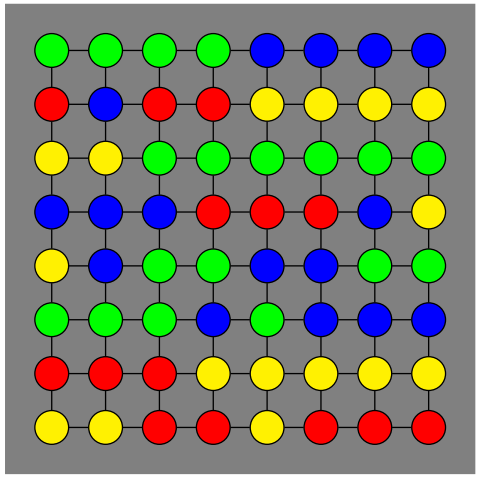
$8 \times 8 \times 8$ Laplacian partitioned using SCOTCH and k-way clustering on the first separator

Clustering techniques: existing solutions

- k-way partitioning (dense, multifrontal)
- Supernode reordering techniques (supernodal)



(a) Symbolic factorization



(b) First separator clustering

$8 \times 8 \times 8$ Laplacian partitioned using SCOTCH and Reordering clustering on the first separator

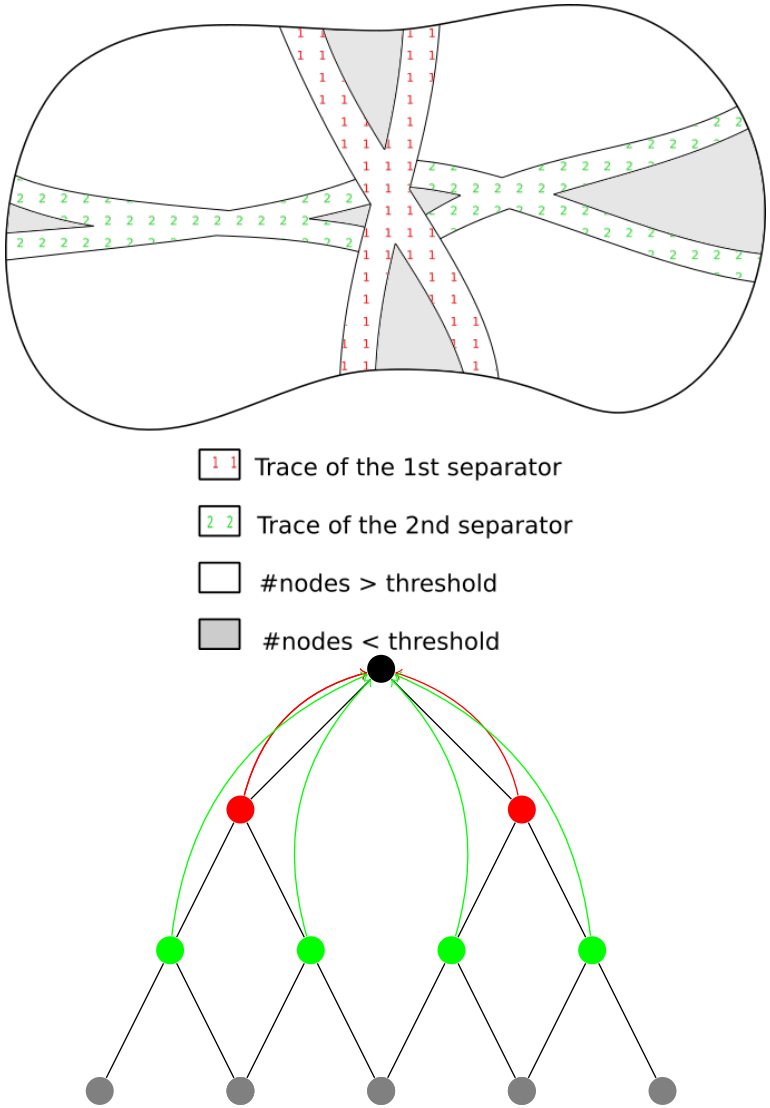
New heuristic based on projections

Pre-selected vertices of a separator are vertices connected to a close child in the elimination tree

For each separator we have:

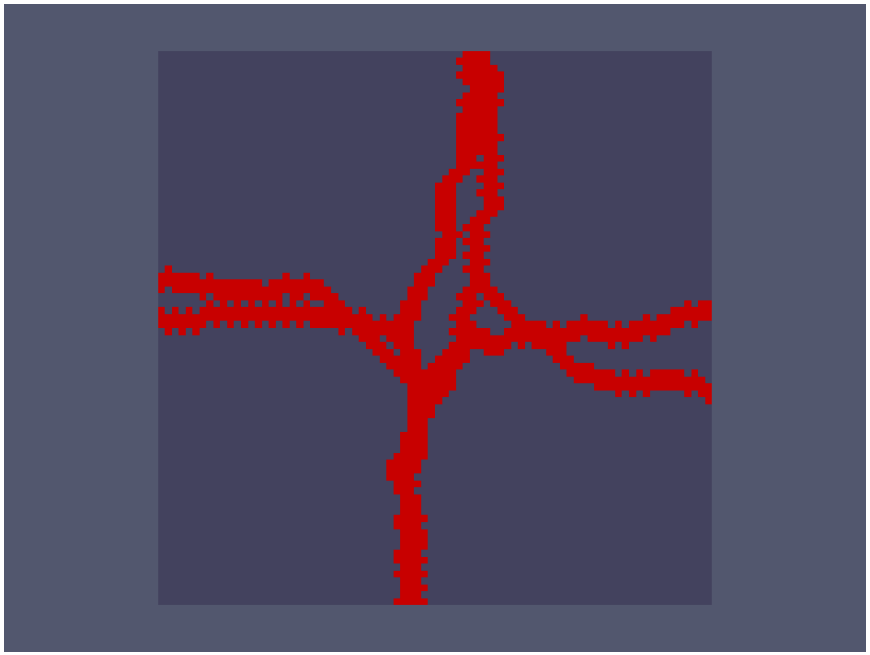
$$A_{22} = \begin{pmatrix} A_{kk} & A_{ks} \\ A_{sk} & A_{ss} \end{pmatrix}$$

where A_{ss} corresponds to pre-selected vertices.
Only interactions between non pre-selected vertices A_{kk} are compressed



Example - $80 \times 80 \times 80$ Laplacian matrix

Interactions with pre-selected vertices (in red) are not compressed



Projections heuristic on last separator of size 80×80

1. Compute pre-selected vertices

Example - $80 \times 80 \times 80$ Laplacian matrix

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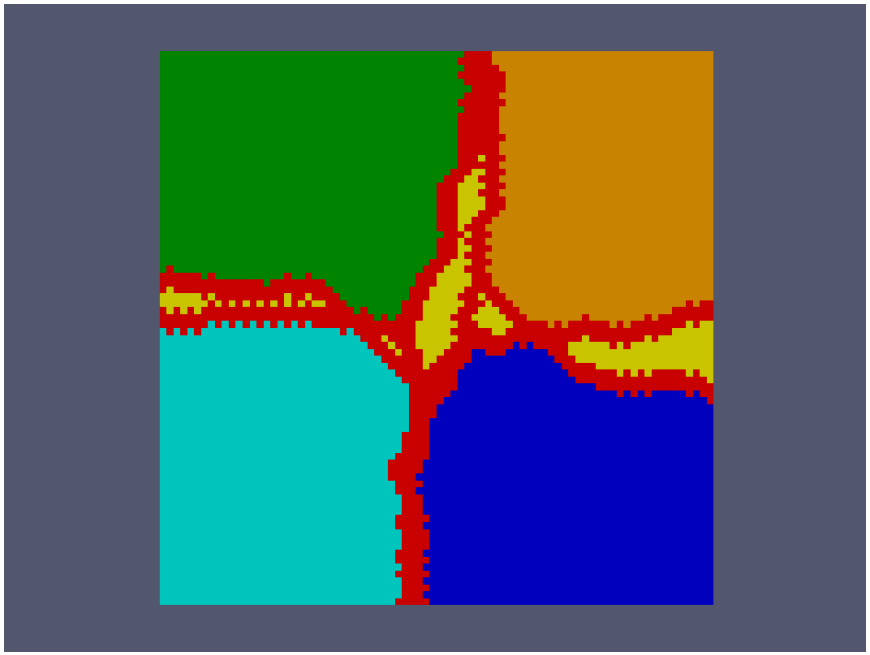

Projections heuristic on last separator of size 80×80

1. Compute pre-selected vertices
2. Isolate connected components
3. Merge small components

Example - $80 \times 80 \times 80$ Laplacian matrix

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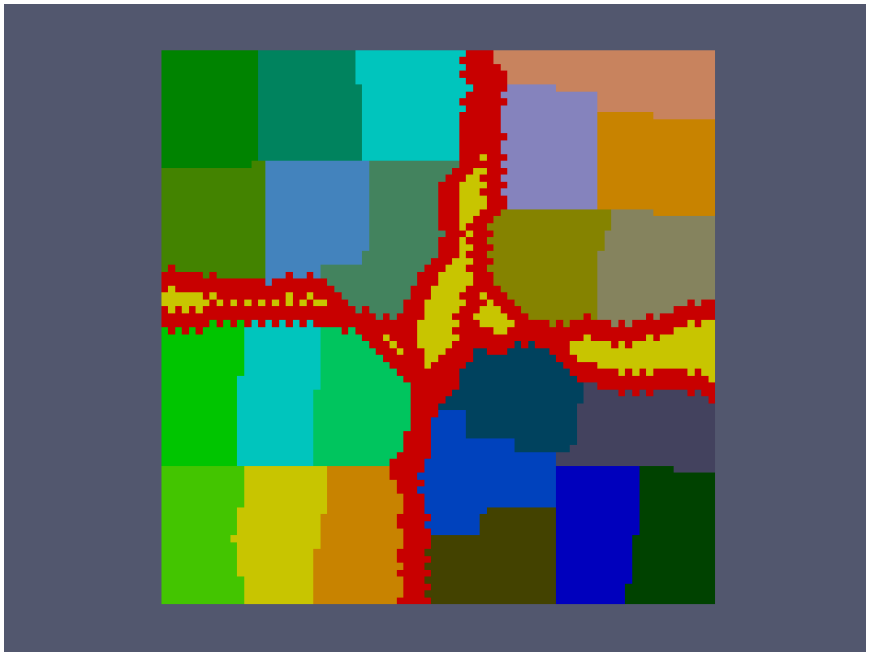


Projections heuristic on last separator of size 80×80

1. Compute pre-selected vertices
2. Isolate connected components
3. Merge small components
4. Apply k-way partitioning on large components
5. Perform TSP reordering on each cluster

Experimental setup

Architecture

- 2 INTEL Xeon $E5-2680v3$ at 2.50 GHz
- 128 GB
- 24 threads

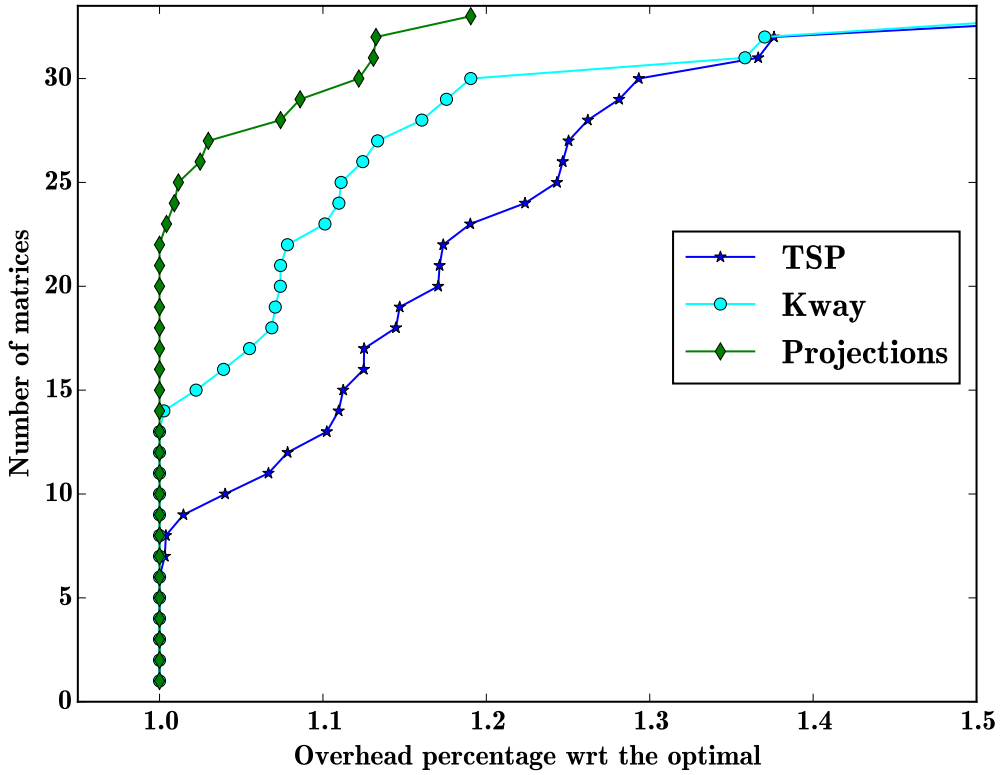
Set of matrices

- 33 square matrices from the SuiteSparse Matrix Collection
- real or complex
- $50K \leq N \leq 5M$
- $nb_{ops} > 1$ TFlops

Strategies studied for the PaStiX solver

- Reordering with TSP
- K-way partitioning using SCOTCH + TSP on each cluster
- The new Projections strategy + TSP on each cluster

Performance profile of the factorization time

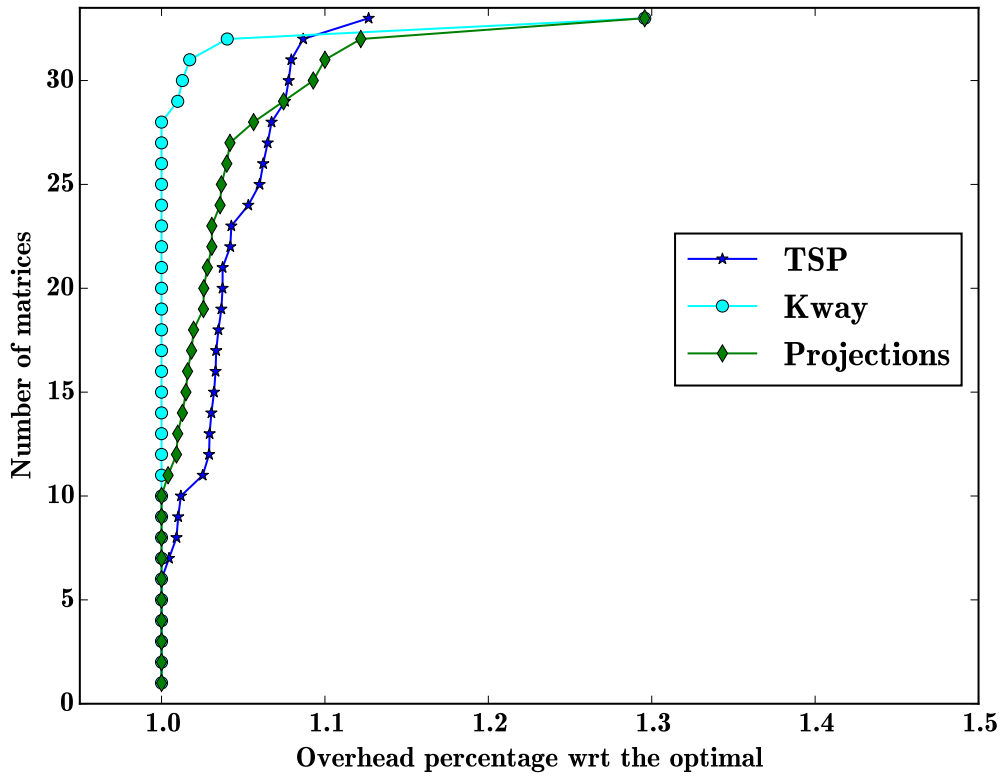


Method

- For each matrix, percentage wrt the best method
- Percentage are sorted increasingly
- A curve close to $x = 1$ is close to optimal

Minimal Memory (fully structured with low-rank updates), with $\tau = 10^{-8}$

Performance profile of the memory consumption



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Minimal Memory (fully structured with low-rank updates), with $\tau = 10^{-8}$

Clustering summary

Ordering strategies

- Both reordering and k-way are limited to form suitable clusters
- Pre-selection of some unknowns allows to obtain well-separated clusters and to exhibit non-compressible operations

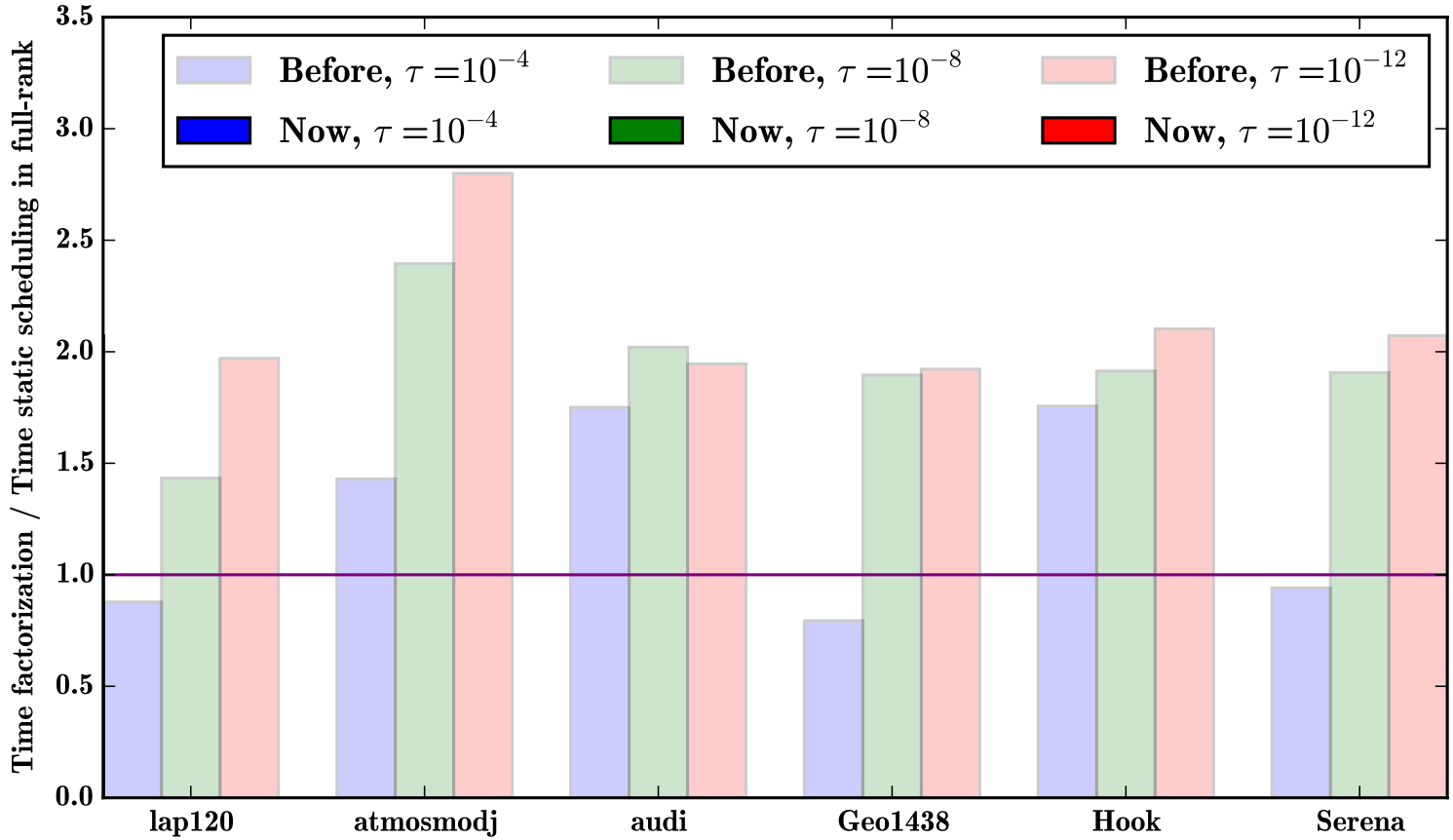
Impact on preprocessing stats

- Ordering time controlled: 70% overhead with respect to SCOTCH ordering
- Slight increase in the number of off-diagonal blocks: mean 1.05, max 1.35 for both **K-way** and **Projections** strategies

Conclusion

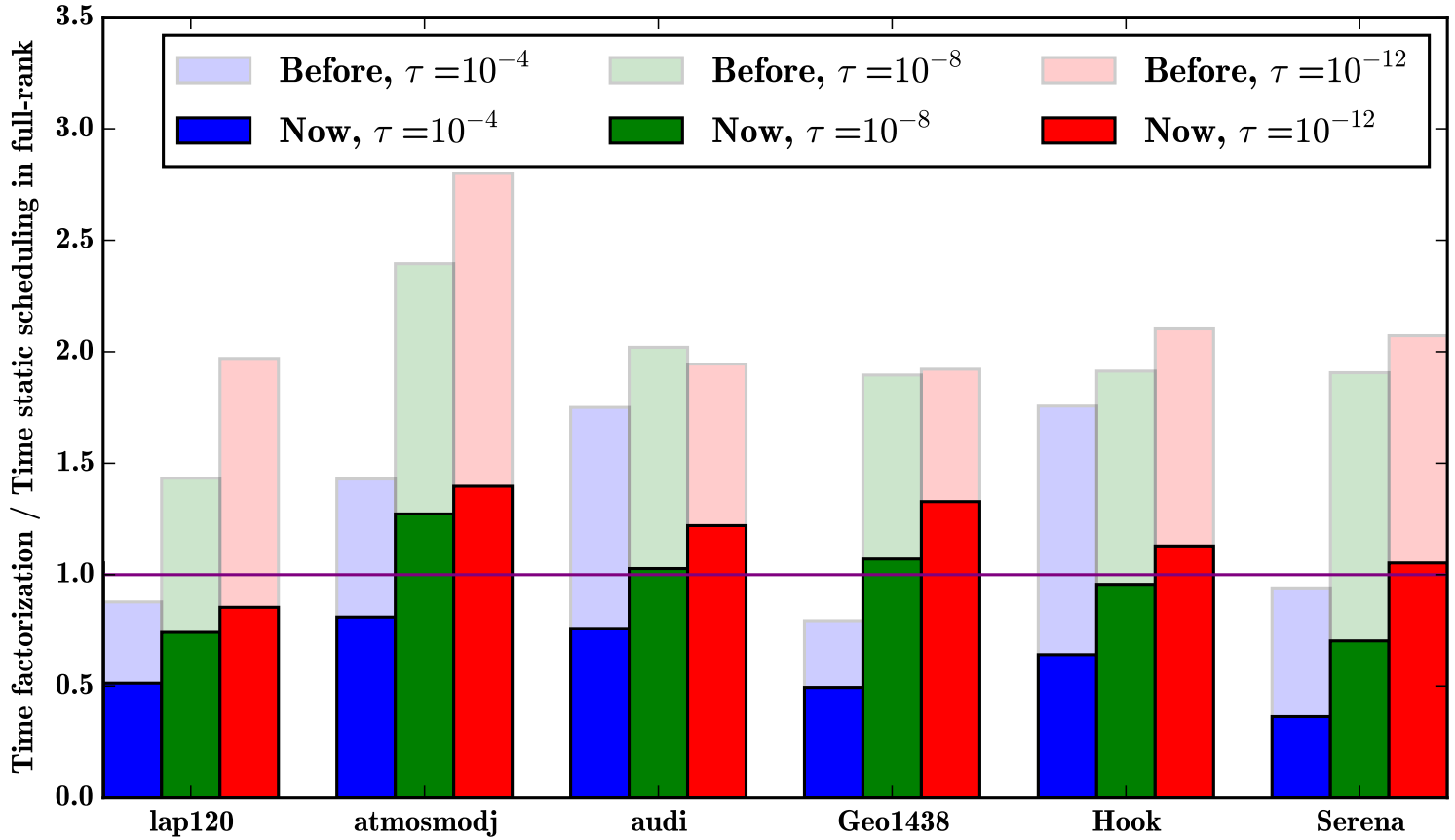
- Somewhat similar to ILU(k) to select more important data
- When moving to hierarchical matrices, the cluster trees may not be binary trees

Behavior of RRQR/Minimal Memory with PaRSEC and Projections



Adding Projections and the use of PaRSEC runtime system reduces factorization time

Behavior of RRQR/Minimal Memory with PaRSEC and Projections



Adding Projections and the use of PaRSEC runtime system reduces factorization time

HORSE: Practical application (S. Lanteri - ANR TECSER)

Method

- Introduce an hybrid variable to solve a system smaller than the one obtained through DG
- Perform Domain-Decomposition to solve this system
- Use a direct solver for subdomains

Solve 3D frequency-domain Maxwell's equations

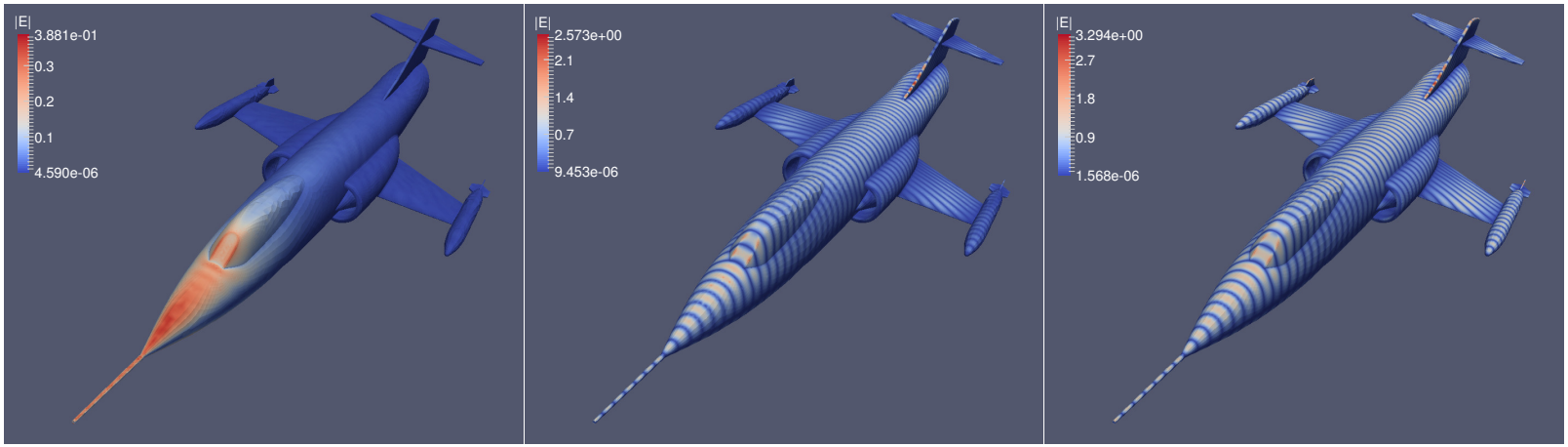
- $\mathbf{i}\omega\varepsilon_r\mathbf{E} - \mathbf{curl}\,\mathbf{H} = -\mathbf{J},$ in Ω
- $\mathbf{i}\omega\mu_r\mathbf{H} + \mathbf{curl}\,\mathbf{E} = 0,$ in Ω
- $\mathbf{n}\times\mathbf{E} = 0,$ on Γ_m
- $\mathbf{n}\times\mathbf{E} + \mathbf{n}\times(\mathbf{n}\times\mathbf{H}) = \mathbf{n}\times\mathbf{E}^{\text{inc}} + \mathbf{n}\times(\mathbf{n}\times\mathbf{H}^{\text{inc}}),$ on Γ_a

HORSE: Hybridizable DG method in 3D

Scattering of a plane wave by a jet

- Unstructured tetrahedral mesh: $1,645,874$ elements / $3,521,251$ faces
- Frequency: 600 MHz, Wavelength: $\lambda \simeq 0.5$ m, Penalty parameter: $\tau = 1$

HDG method	# DoF $\mathbf{\Lambda}$ field	# DoF EM field
HDG-$\mathbb{P}_1$	21,127,506	39,500,976
HDG-$\mathbb{P}_2$	42,255,012	98,752,440
HDG-$\mathbb{P}_3$	70,425,020	197,504,880



Contour line of $|\mathbf{E}|$ - HDG$-\mathbb{P}_1$ to HDG$-\mathbb{P}_3$

Experimental setup

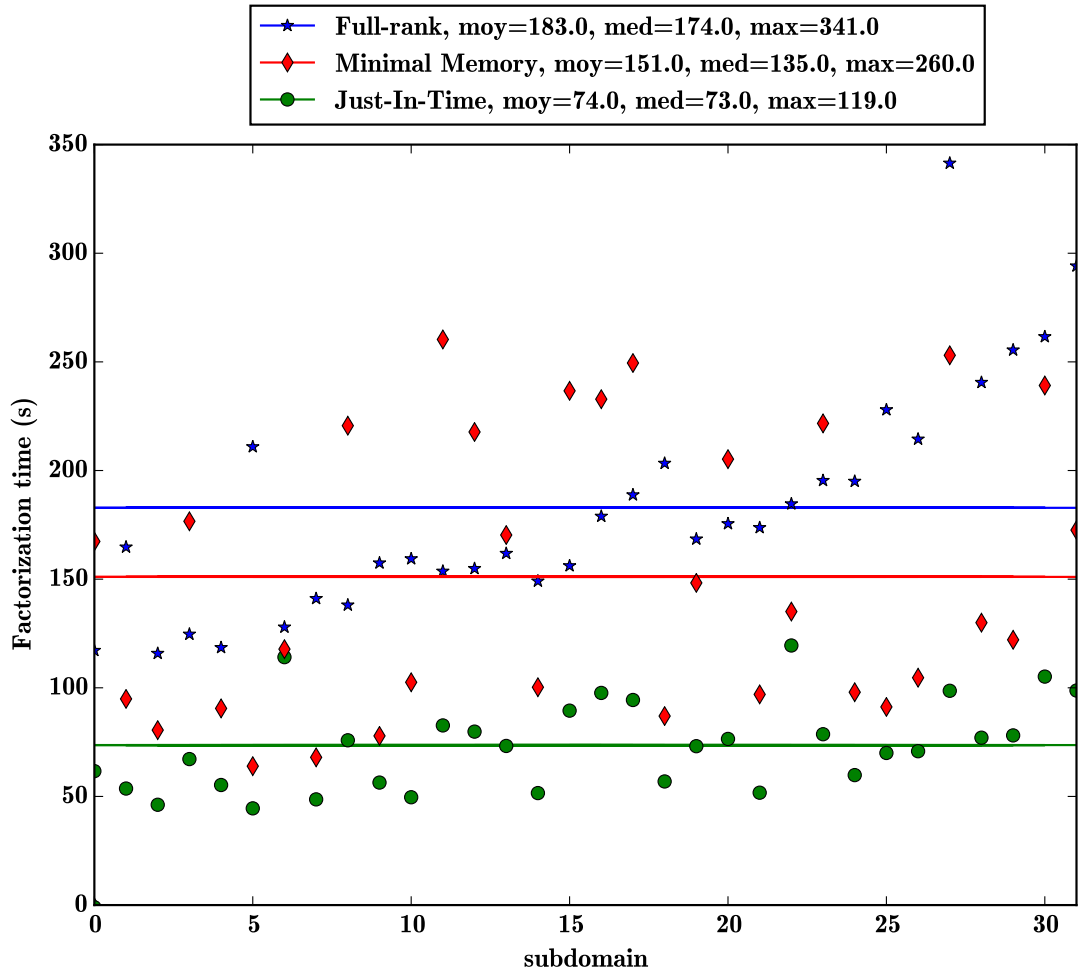
Study case

- Jet with $\mathbb{P}_2$ interpolation
- $42\ 255\ 012$ unknowns for $\mathbf{\Lambda}$
- A single factorization is performed on each subdomain
- There may be several solves for iterative refinement between subdomains

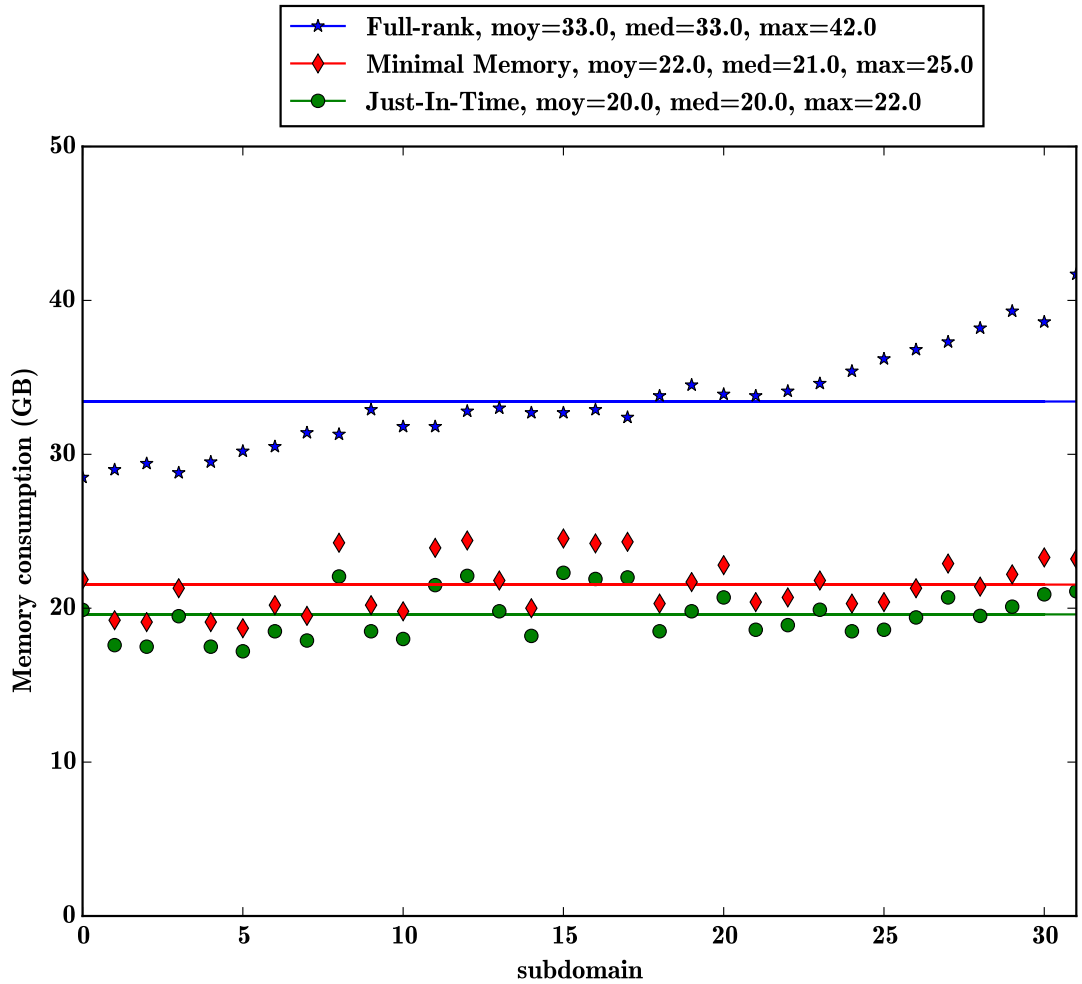
Machine

- Occigen: 24-cores nodes with 128 GB
- Each MPI process is hold on a socket with 12 cores
- In next experiments, we use 32, 48 or 64 subdomains
- Subdomains are ordered accordingly to the number of operations for the complete factorization

Factorization on each subdomain – 32 processes with $\tau = 1e-4$



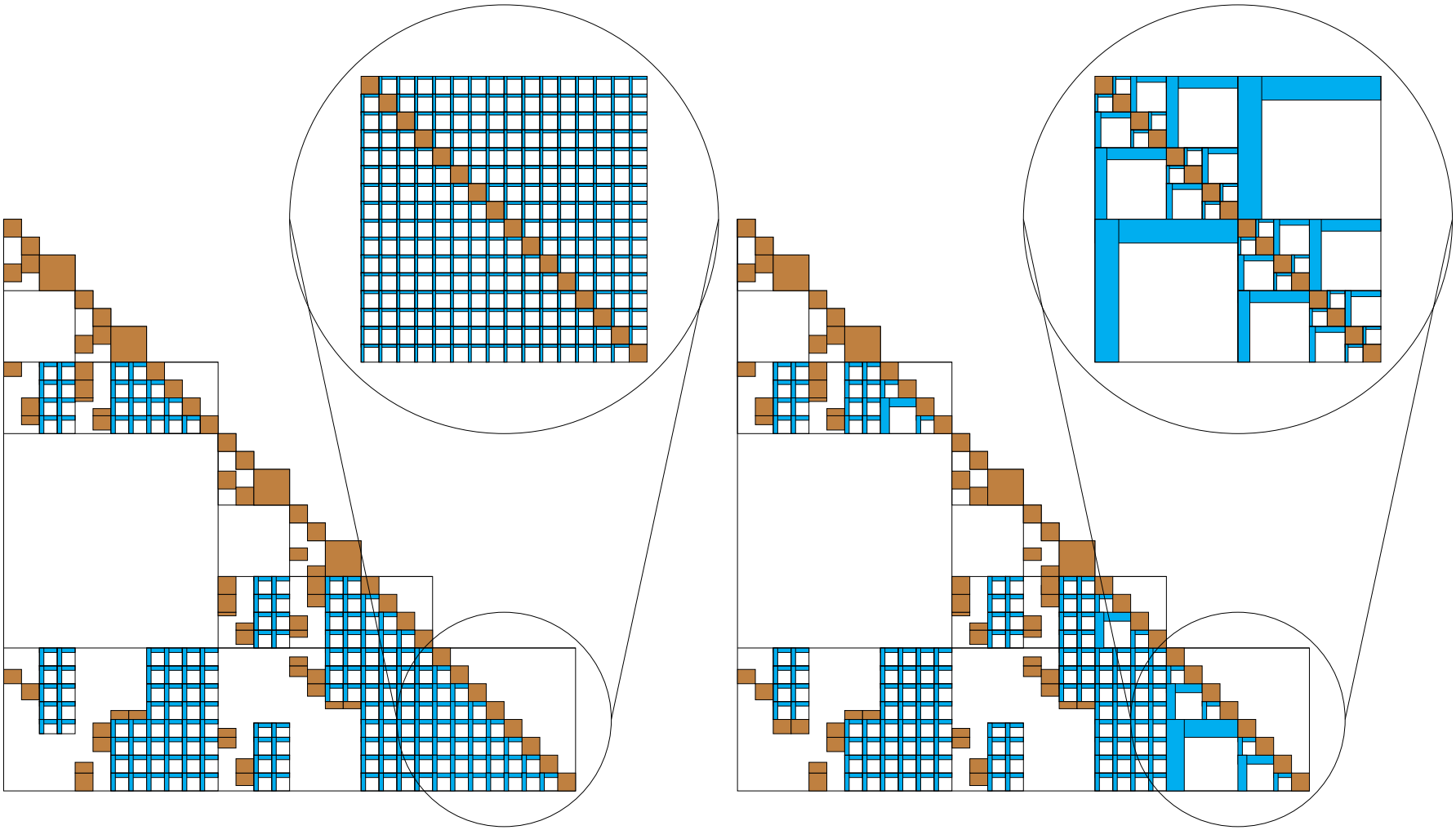
Memory Consumption on each subdomain – 32 processes with $\tau = 1e-4$



Impact on HORSE

Subs	τ	Method	Fact(s)	Nb. of iters	Refinement (s)	HDGM (s)	Memory (GB)
32	-	Full-rank	526.0	9	254.5	814.0	41.7
	1e-4	Just-In-Time	209.3	9	164.8	**405.8**	41.7 (22.3)
		Minimal-Memory	516.7	15	273.2	822.0	**24.5**
	1e-8	Just-In-Time	325.2	9	192.9	550.4	41.7 (29.4)
		Minimal-Memory	600.1	9	193.2	825.8	30.5
48	-	Full-rank	237.3	8	118.6	374.6	24.9
	1e-4	Just-In-Time	112.2	9	106.1	**237.1**	24.9 (14.1)
		Minimal-Memory	229.3	13	159.7	407.5	**15.3**
	1e-8	Just-In-Time	171.5	8	105.8	296.1	24.9 (18.1)
		Minimal-Memory	319.4	8	109.8	447.9	18.8
64	-	Full-rank	179.8	9	104.7	298.3	17.4
	1e-4	Just-In-Time	79.7	10	91.1	**184.1**	17.4 (10.0)
		Minimal-Memory	138.1	13	120.7	272.2	**11.0**
	1e-8	Just-In-Time	124.6	9	90.0	228.2	17.4 (12.9)
		Minimal-Memory	239.2	9	91.5	344.5	13.7

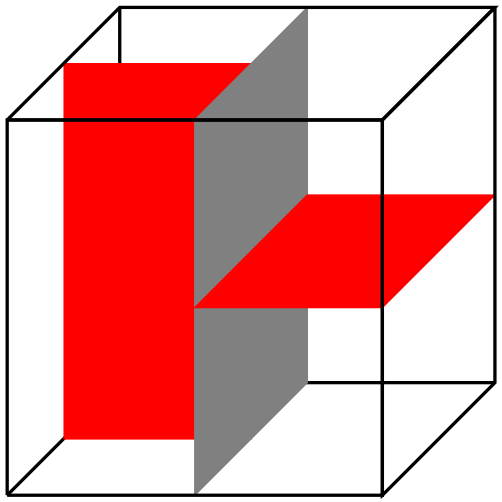
Future works: HODLR compression

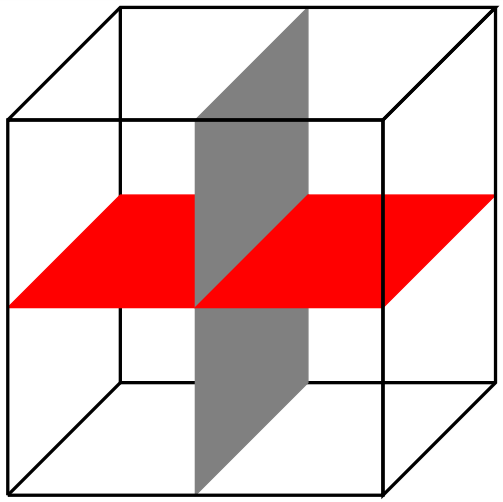


Future works: align separators

Contraint partitioning process

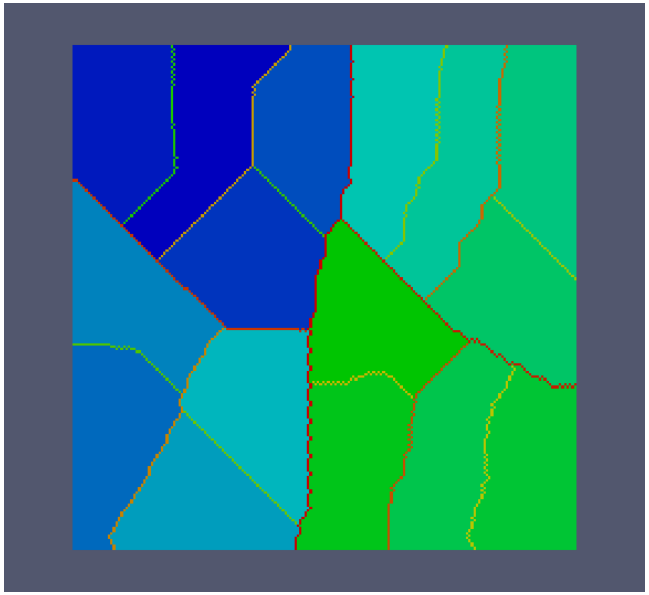
- Align separators to form clusters during the nested dissection process
- Preliminary work using fixed vertices
- When partitioning $G = A \cup B \cup C$, ensure that the children interaction with C is symmetric to have similar contribution pattern



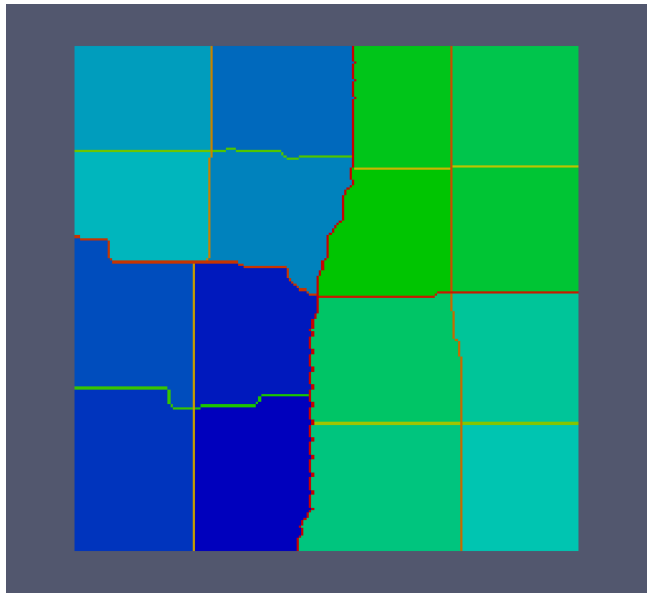


Result on a 200^2 Laplacian

With SCOTCH



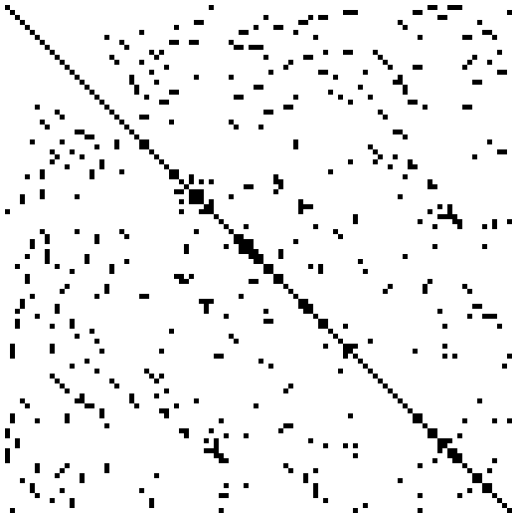
With **ALIGnATOR**



PaStiX 6.0.1

http://gitlab.inria.fr/solverstack/pastix

- Support shared memory with different schedulers:
  - sequential
  - static scheduler
  - PaRSEC/StarPU runtime systems with experimental GPU support
- Low-rank support integrated in master branch with clustering strategies
- Cholesky, LDL and LU factorizations
- GMRES, CG, BiCG iterative refinements



LR2LR kernel using SVD

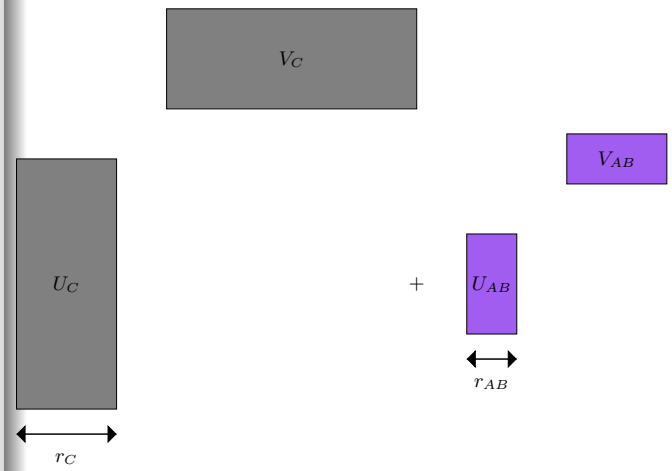
A low-rank structure $U_C V_C^t$ receives a low-rank contribution $U_{AB} V_{AB}^t$

Recompression algorithm

$$U_C V_C^t + U_{AB} V_{AB}^t = \left([U_C, U_{AB}]\right) \times \left([V_C, V_{AB}]\right)^t$$

- QR: $[U_C, U_{AB}] = Q_1 R_1$
- QR: $[V_C, V_{AB}] = Q_2 R_2$
- SVD: $R_1 R_2^t = u \sigma v^t$

$$A = \left(Q_1 u \sigma\right) \times \left(Q_2 v\right)^t$$



The complexity of this operation depends on the dimensions of the target C

Slightly more complex algorithm for RRQR, that still requires zeroes padding

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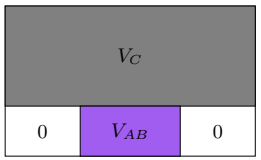

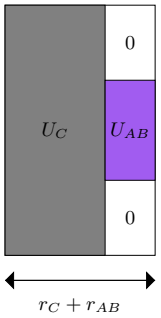

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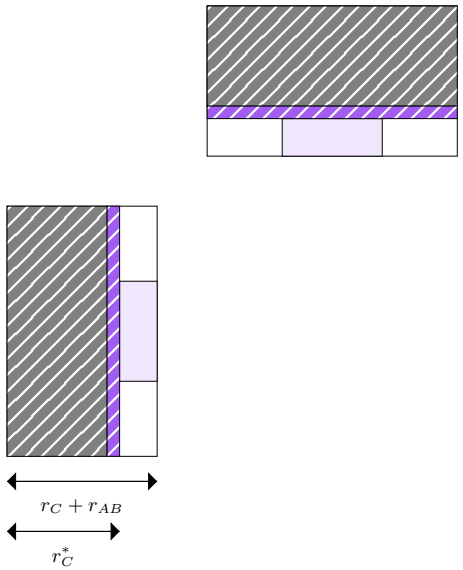


The complexity of this operation depends on the dimensions of the target C

Slightly more complex algorithm for RRQR, that still requires zeroes padding

LR2LR kernel using RRQR

A low-rank structure $u_1 v_1^t$ receives a low-rank contribution $u_2 v_2^t$.
u_1 and u_2 are orthogonal matrices

Algorithm

$$A = u_1 v_1^t + u_2 v_2^t = \left([u_1, u_2]\right) \times \left([v_1, v_2]\right)^t$$

Orthogonalize u_2 with respect to u_1 :

$$u_2^* = u_2 - u_1(u_1^t u_2) \quad \Theta(m r_1 r_2)$$

Form new orthogonal basis, and normalize each column :

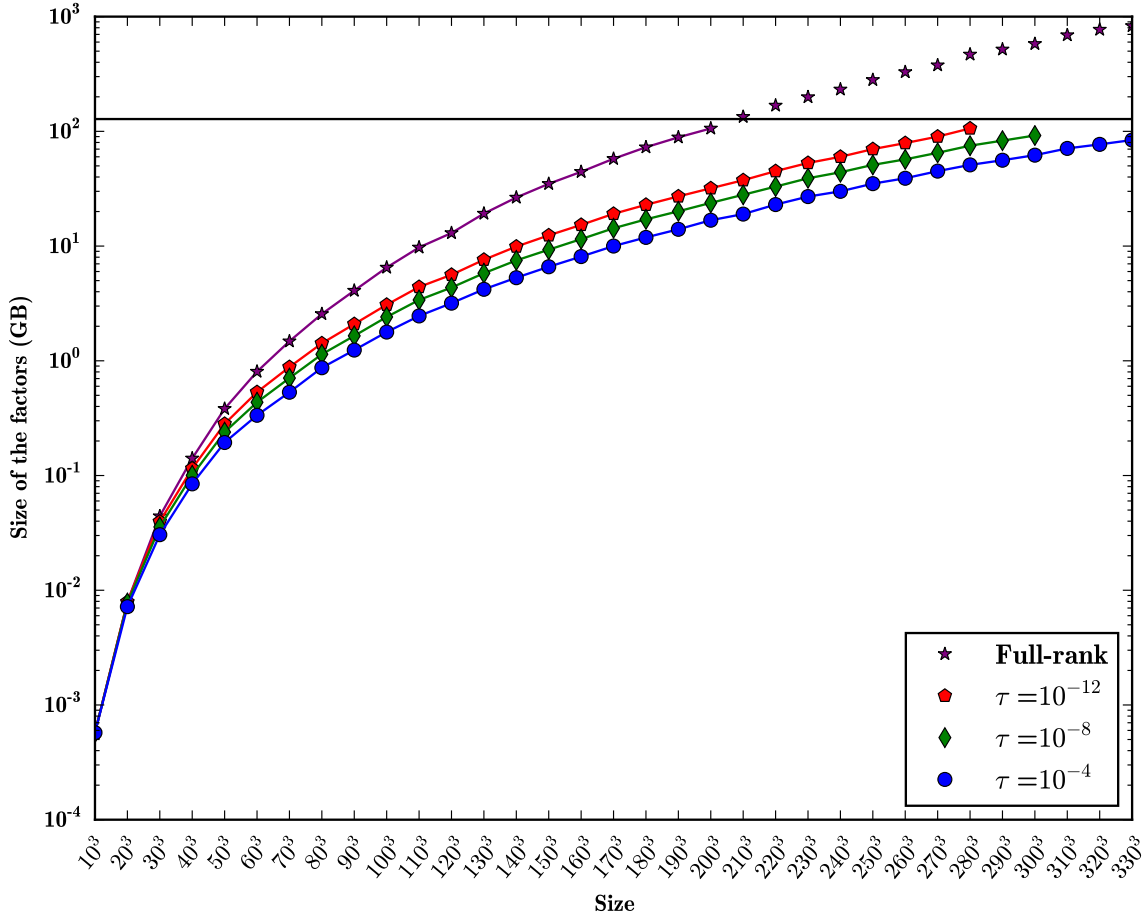
$$[u_1, u_2] = [u_1, u_2^*] \times \begin{pmatrix} I & u_1^t u_2 \\ 0 & I \end{pmatrix}$$

Apply a RRQR on :

$$\begin{pmatrix} I & u_1^t u_2 \\ 0 & I \end{pmatrix} \times \left([v_1, v_2]\right)^t$$

RRQR with truncation in $\Theta(n(r_1 + r_2)r_1^*)$. Less stable?

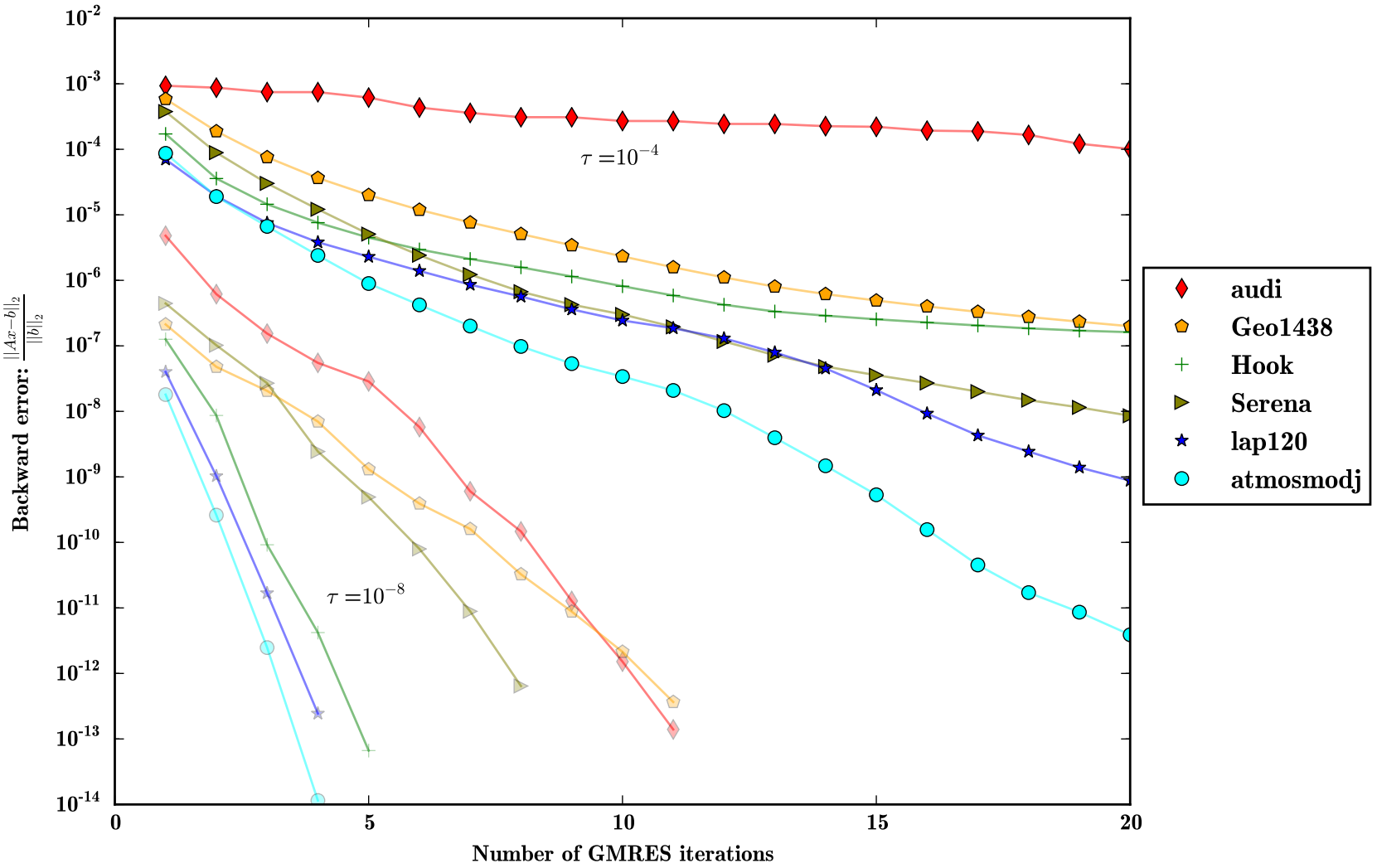
Scaling on Laplacians: memory consumption RRQR/Minimal Memory



Results

- Maximum consumption of 128 GB
- Problem of size $200^3 = 8M$ with full-rank
- Problem of size $330^3 = 36M$ with 10^{-4} tolerance

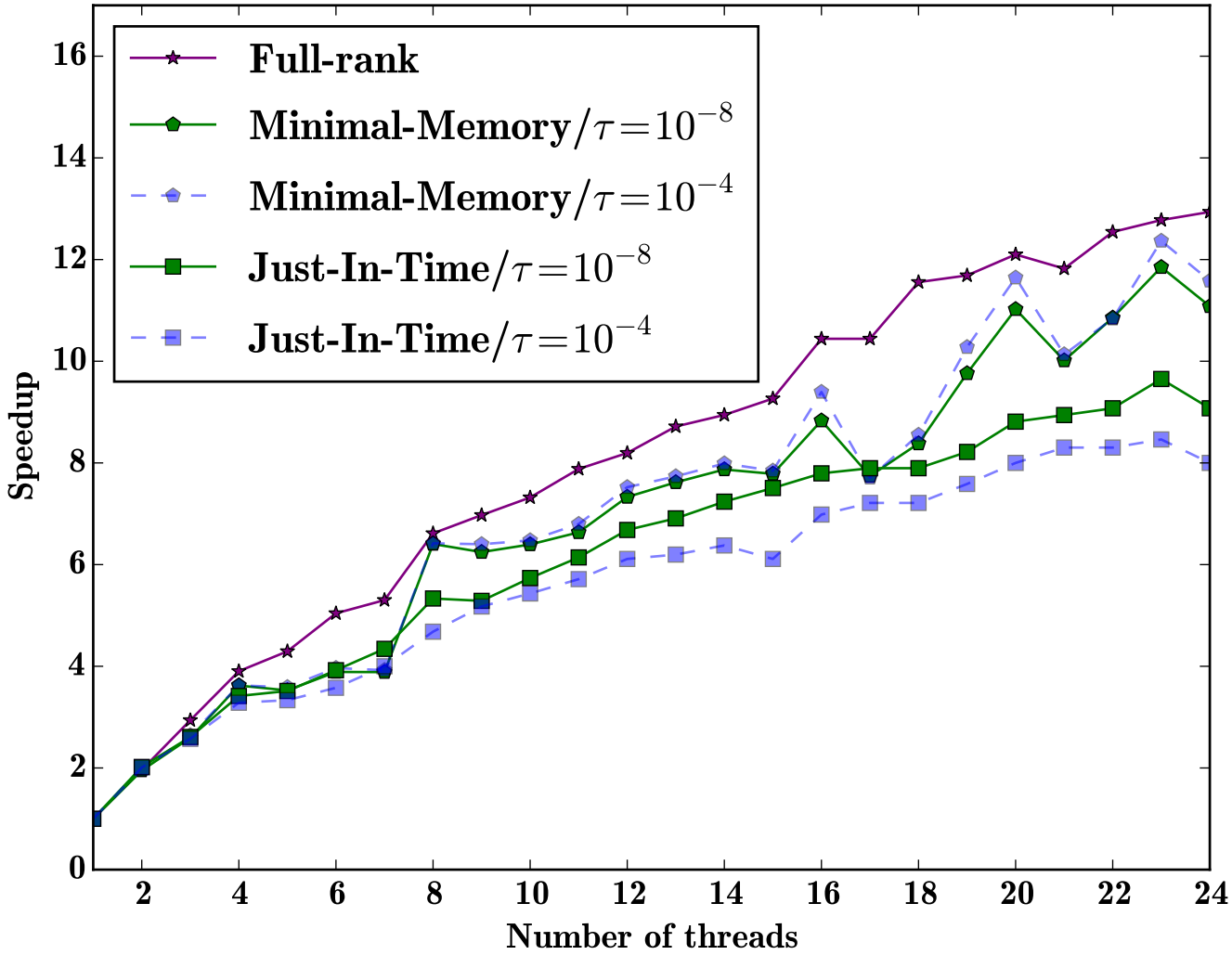
Convergence of RRQR/Minimal Memory



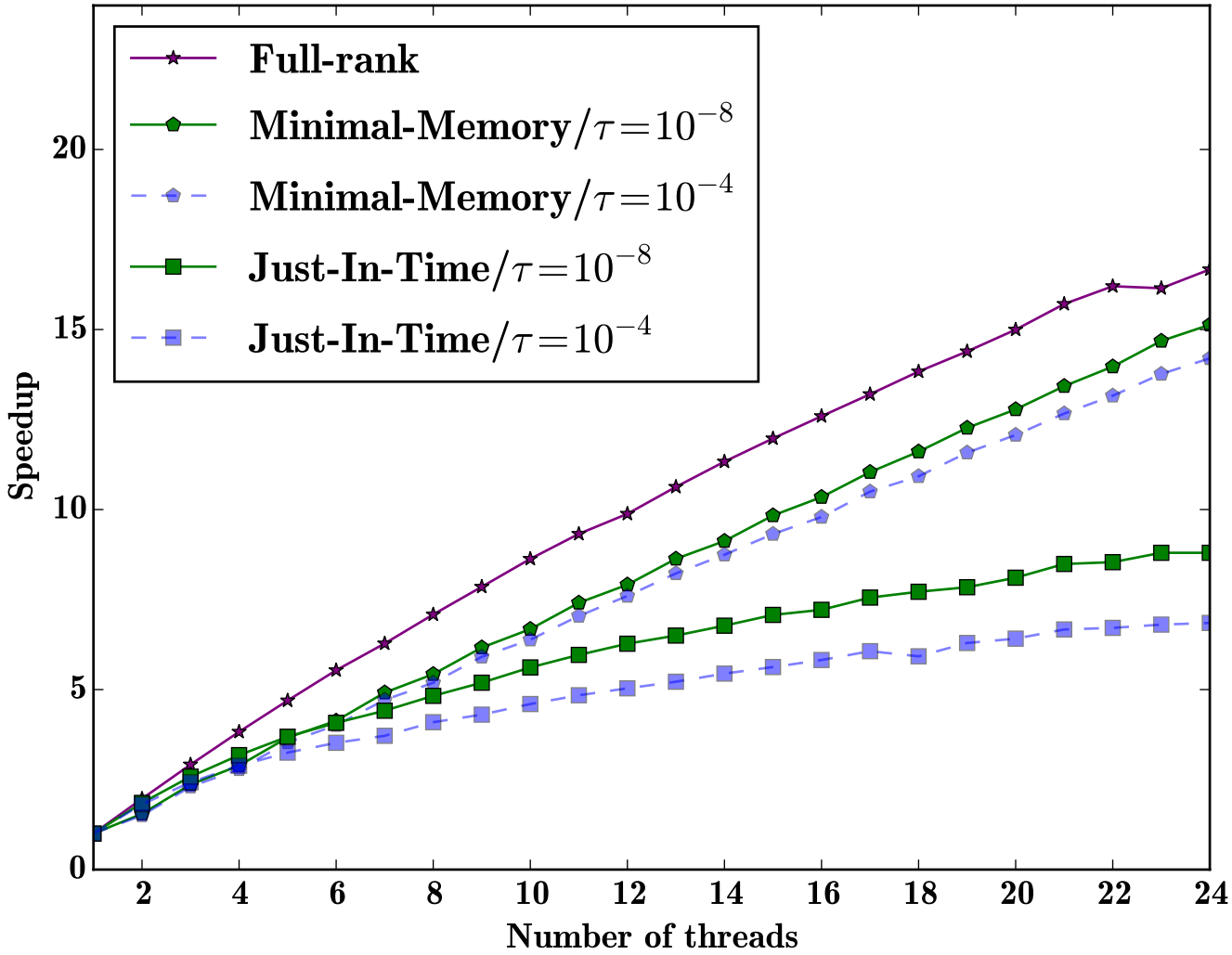
Costs distribution on the Atmosmodj matrix with $\tau = 10^{-8}$

	Full-rank	Just-In-Time		Minimal Memory	
		SVD	RRQR	SVD	RRQR
Factorization time (s)					
Compression	-	4.1e+02	3.4e+01	1.8e+02	5.6+00
Block factorization (GETRF)	7.2e-01	7.4e-01	7.3e-01	7.8e-01	7.6e-01
Panel solve (TRSM)	1.7e+01	6.9e+00	7.4e+00	7.6e+00	7.9e+00
Update					
Formation of contribution	-	-	-	9.9e+01	4.2e+01
Addition of contribution	-	-	-	3.0e+03	7.3e+02
Dense udpate (GEMM)	4.6e+02	1.3e+02	9.7e+01	2.8e+01	2.4e+01
Total	**4.7e+02**	**5.5e+02**	**1.4e+02**	**3.6e+03**	**8.1e+02**
Solve time (s)	6.3e+00	1.9e+00	3.0e+00	**1.5e+00**	3.2e+00
Factor final size (GB)	16.3	6.95	7.49	**6.85**	7.31
Memory peak for the factors (GB)	16.3	16.3	16.3	**6.85**	7.31

Parallelism / static scheduling



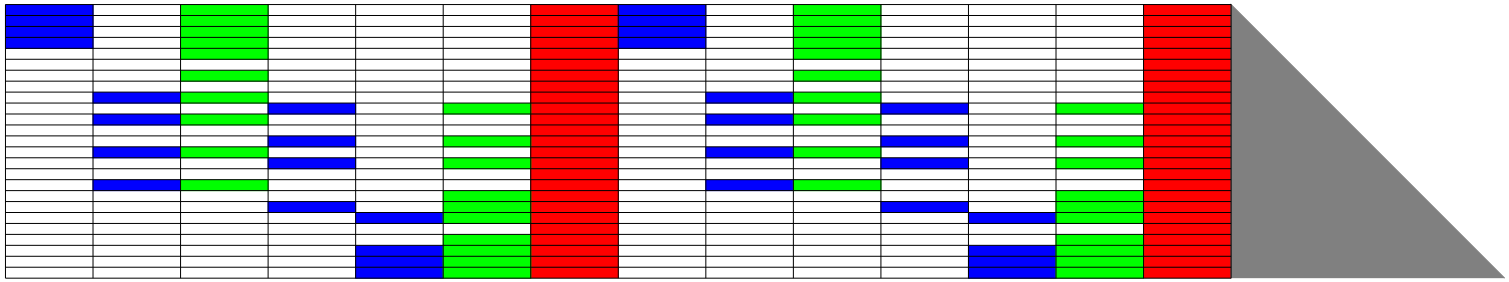
Parallelism / Parsec



Modeling of the problem

Proposition

- Define a distance between rows: the number of differences between off-diagonal blocks
- Express the problem as a Traveling Salesman Problem (TSP) to sort rows in order to minimize the overall distance
- Use heuristics to perform TSP with low complexity



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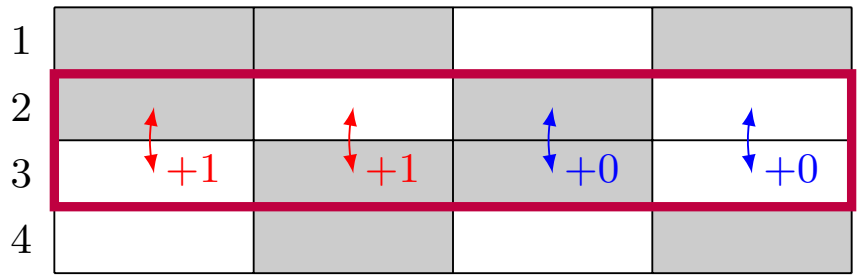


	1	2	3	4
1	0	-	-	-
2	3	0	-	-
3	3	2	0	-
4	1	4	2	0

Improvements with $\tau = 10^{-8}$ on a set of six matrices

Variant	Just-In-Time		Minimal Memory		
	Time PaRSEC	Time static	Time PaRSEC	Time static	Memory
strong admissibility	0.52	0.62	1.24	2.28	0.52
+ k-way	**0.49**	0.55	1.17	1.94	**0.48**
+ projections	0.50	0.55	1.19	1.90	0.50
+ ratio set to 0.5	0.51	0.56	**0.96**	1.43	0.54
+ ratio set to 0.25	0.50	0.55	1.19	1.89	0.50

Towards sparse ordering dedicated to low-rank

Nested dissection

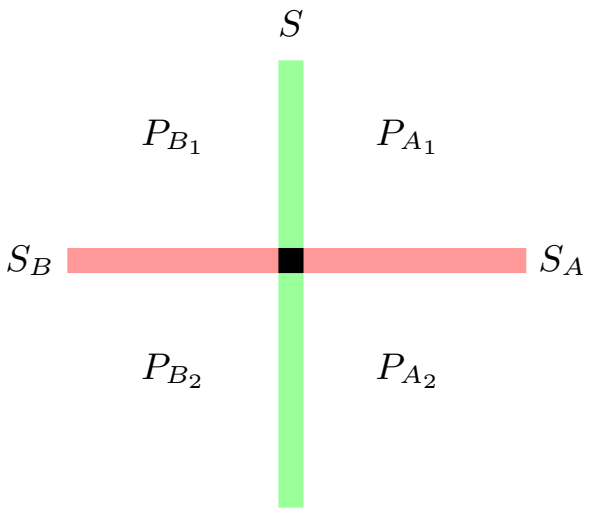
1. Partition $V = A \cup B \cup S$, such as any path from A to B goes through S
2. Order S with larger numbers: $V_A < V_B < V_S$
3. Apply the process recursively on A and B

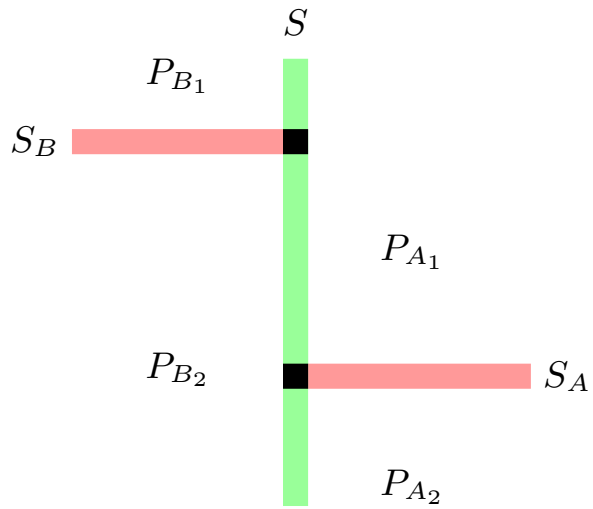
As A and B are processed independently, their contribution on S is not symmetric

Current solutions in sparse low-rank solvers

- Find low-rank clustering by applying a k-way partitioning on each separator (Mumps, Strumpack)
- Reordering strategy to cluster close contributions (PaStiX, and cf. previous talk)

Simple representation of the problem on a 2D graph

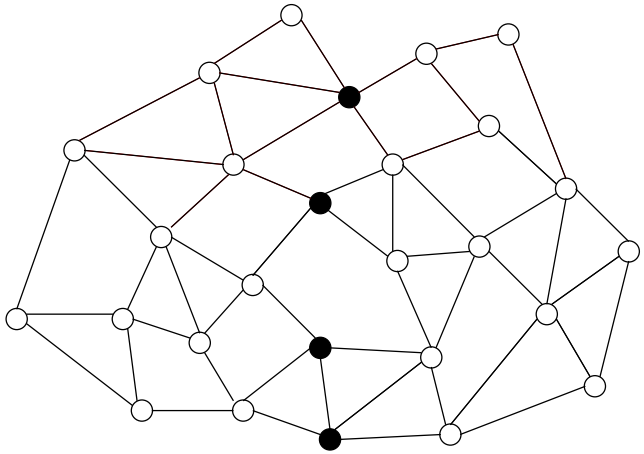




- Single interaction between S and $S_A \cup S_B$ in the original graph
- Two large interaction blocks $P_{A_1} \cup P_{B_1}$ and $P_{A_2} \cup P_{B_2}$ during the factorization

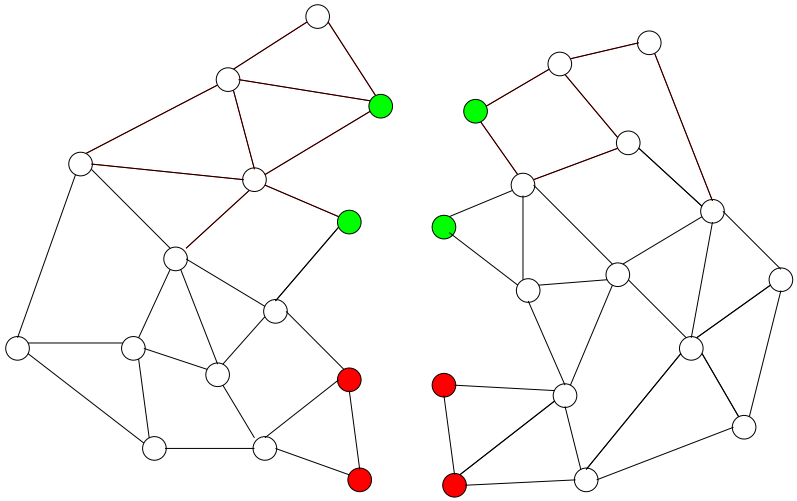
- Double interaction: between S and S_A and between S and S_B in the original graph
- Three “large” interaction blocks during the factorization

Fixed vertices



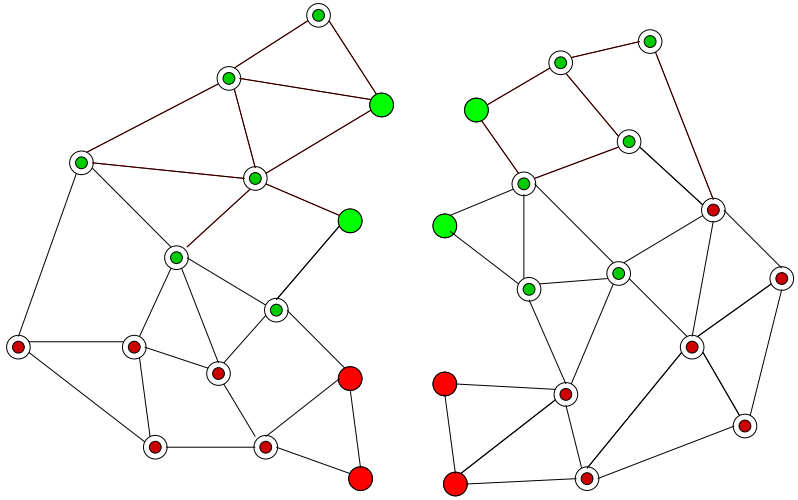
- Regular nested dissection on $G = A \cup B \cup C$.

Fixed vertices



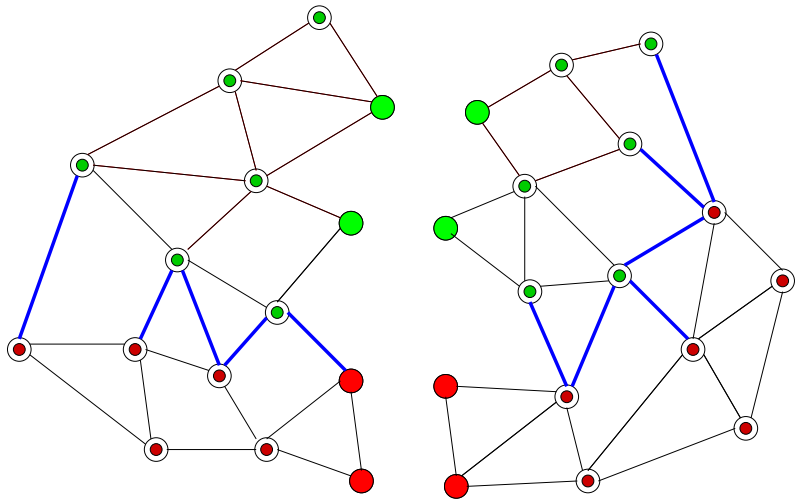
- Recursion with the halo on $A \cup C$ and $B \cup C$.
- C vertices are bi-partitioned into green and red vertices.

Fixed vertices



- The partition of C is extended to both $A \cup C$ and $B \cup C$.

Fixed vertices



- We got a new edge separator for both subgraphs.
- Turn those separators into vertex separators.